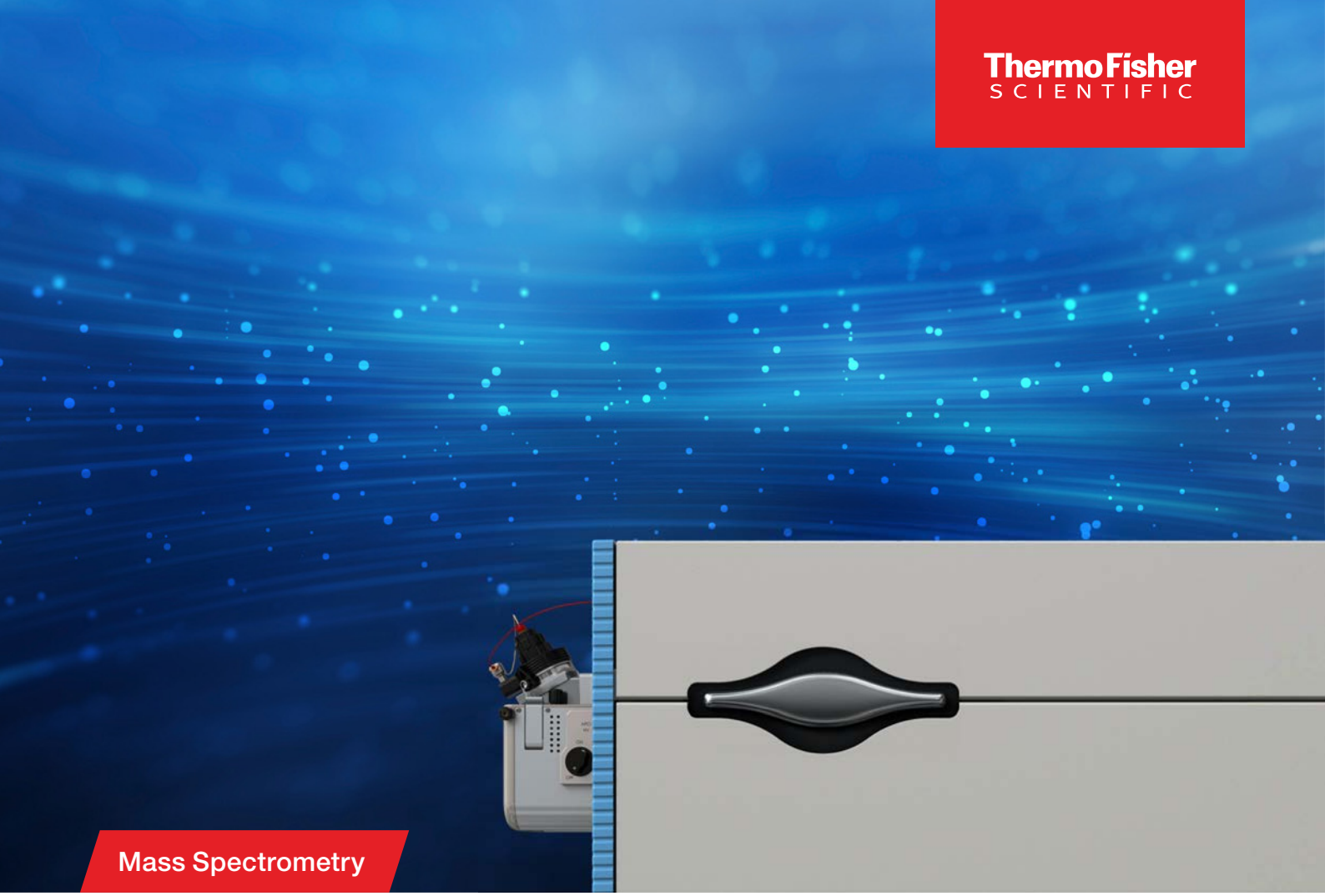


Mass Spectrometry

Orbitrap Exploris MX

Software Manual

BRE0030646 Revision C October 2022

ThermoFisher SCIENTIFIC

Orbitrap Exploris MX

Software Manual

BRE0030646 Revision C October 2022

thermo scientific

Legal Notices

Published by:
Thermo Fisher Scientific (Bremen) GmbH, Hanna-Kunath-Str. 11, 28199 Bremen, Germany
Tel: +49(0)421 5493 0, Fax: +49(0)421 5493 396

Release History: Revision A released in November 2021.
Revision B released in April 2022.
Revision C released in October 2022.

Software Version: Thermo Scientific Orbitrap Exploris Series 4.2 Instrument Control Software

General Lab Equipment, Not for Clinical, Patient or Diagnostic Use.

C

Contents

1

Using this Manual

Welcome to the Thermo Scientific™ Orbitrap Exploris MX system! The Orbitrap Exploris MX mass spectrometer is a member of the Thermo Scientific family of mass spectrometers that are powered by Orbitrap™ technology.

Contents

License for Optional Features

During the installation of the Orbitrap Exploris Series MS, the Thermo Fisher Scientific field service engineer activates the optional purchased licenses.

About this Manual

The *Orbitrap Exploris MX Software Manual* describes software-related operating procedures of the Orbitrap Exploris MX mass spectrometer.

To obtain a good understanding of the complete system, we recommend that you study the *Orbitrap Exploris Series Operating Manual*. This manual also contains extensive information that concerns the safety of the personnel that operate the instrument. A basic knowledge of handling computers and of the Xcalibur™ software is assumed for the correct operation of the Orbitrap Exploris Series system.

Designed, manufactured and tested in an ISO9001 registered facility, this instrument has been shipped to you from our manufacturing facility in a safe condition. This instrument must be used as described in this manual. Any use of this instrument in a manner other than described here may result in instrument damage and/or operator injury.

Typographical Conventions

This section describes typographical conventions that have been established for Thermo Fisher Scientific manuals.

Signal Words

Make sure that you follow the precautionary statements presented in this manual. The special notices appear different from the main flow of text:

NOTICE Points out possible material damage and other important information in connection with the instrument.

Tip Highlights helpful information that can make a task easier.

Viewpoint Orientation

The expressions *left* and *right* used in this manual always refer to the viewpoint of a person that is facing the front side of the instrument.

Data Input

Throughout this manual, the following conventions indicate data input and output via the computer:

- Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
- Input that you enter by keyboard is identified by quotation marks: single quotes for single characters, double quotes for strings.
- For brevity, expressions such as "choose **File > Directories**" are used rather than "pull down the File menu and choose Directories."
- Any command enclosed in angle brackets < > represents a single keystroke. For example, "press **<F1>**" means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, "press **<Shift>** + **<F1>**" means press and hold the <Shift> key and then press the <F1> key.
- Any button that you click on the screen is represented in bold face letters. For example, "click **Close**."

Topic Headings

The following headings are used to show the organization of topics within a chapter:

Chapter Name

Second Level Topics

Third Level Topics

Fourth Level Topics

Reference Documentation

In addition to this guide, Thermo Fisher Scientific provides the following documents for the Orbitrap Exploris MX mass spectrometer:

- *Orbitrap Exploris Series Pre-Installation Requirements Guide*

  This manual contains information on the required environmental conditions in the intended location for the instrument.

- *Orbitrap Exploris Series Operating Manual*

  This manual contains precautionary statements that can prevent personal injury and instrument damage. It also describes the modes of operation and principle hardware components of the instrument. In addition, this manual provides step-by-step instructions for cleaning and maintaining the instrument.

- *Orbitrap Exploris Performance Maintenance Manual*

  This manual describes the user maintenance for the quadrupole and the bent flatapole.

You can access PDF files of the documents listed above and of this manual from the data system computer. The software also provides Help.

❖ **To view product manuals**

From the Microsoft™ Windows™ taskbar, choose **Start > All Apps > Thermo Instruments** (or **Thermo *model***), and then open the applicable PDF file.

Refer also to the user documentation provided by the manufacturers of third party components:

- Forepumps
- Turbomolecular pumps
- Vacuum gauges
- Data system computer and monitor
- Safety data sheets

Contacting Us

There are several ways to contact Thermo Fisher Scientific. You can use your smartphone to scan a QR Code, which opens your email application or browser.

Contact	Link / Remarks	QR Code
Brochures and Ordering Information	www.thermofisher.com/orbitrap	
AnalyteGuru	Planet Orbitrap has migrated into the AnalyteGuru.com community. With this, the existing planetorbitrap.com website will be fully decommissioned, and the existing Planet Orbitrap content has been redirected. To continue to have access to existing and new resources, you will need to register for a new account on AnalyteGuru.com. Because the Planet Orbitrap content has expanded into a community model, some common items from Planet Orbitrap have changed. To help bridge these gaps, AnalyteGuru created guides on how to search the community and how to subscribe to tailored content updates that are available under the Welcome Planet Orbitrap Members website (www.analyteguru.com/t5/Knowledgebase/Welcome-Planet-Orbitrap-Members/ta-p/13999). This dedicated community support section will help getting started with AnalyteGuru.	
Service Contact	For technical support related to your instrument or software, visit the **Services & Support** tab at www.thermofisher.com or visit www.unitylabservices.com to find the customer care telephone line or email address for your geographical region.	
Technical Documentation SharePoint	❖ **To get user manuals for your product** 1. With the serial number (S/N) of your instrument,* request access on our customer SharePoint as a customer at www.thermofisher.com/Technicaldocumentation 2. For the first login, you have to create an account. Follow the instructions given on screen. Accept the invitation within six days and log in with your created Microsoft™ password. 3. Download current revisions of user manuals and other customer-oriented documents for your product. Translations into other languages may be available there as well. * You can find the serial number of your instrument on the name plate. Refer to the *Orbitrap Exploris Series Operating Manual* for the location.	

Contact	Link / Remarks	QR Code
Customer Feedback	❖ **To suggest changes to this manual** You are encouraged to report errors or omissions in the manual. Send an email to the Technical Documentation at documentation.bremen@thermofisher.com. The PDF versions of our manuals allow adding comments with Adobe Acrobat Reader or other freely available PDF reader programs.	

2

Configuring the Instrument in Thermo Foundation

To establish control of the mass spectrometer from the data system computer, use the Thermo Foundation™ Instrument Configuration window to configure the instrument.

Tip The Instrument Configuration window displays all changed set values of given parameters in bold type until you click OK or Apply. To enable the new settings, restart the data system computer.

❖ **To configure the mass spectrometer in the Foundation Instrument Configuration window**

1. From the Windows taskbar, choose **Start > All Apps > Thermo Foundation *x.x* > Instrument Configuration**, where *x.x.* is the installed version.
2. Add the mass spectrometer's icon to the list of Configured Devices, and then configure the mass spectrometer parameters.
3. Click **Done**.

Parameters in the Instrument Configuration Window

Parameter	Description
System Information	
Model	Displays the mass spectrometer model name.
Serial Number	Displays the serial number of the instrument.
Instrument Name	(Optional) The name for the instrument.
Inlet	
Divert Valve	• None (for no divert valve) (Default) • A (for a system with one divert valve) • A and B (for a system with two divert valves)
Syringe Pump	Configured: Indicates that the system includes a data-system controlled syringe pump. Default: Not Configured

Parameter	Description
Contact Closure	Select the event type that triggers the contact closure: • Transition close-to-open (Default) • Transition open-to-close
Wait for Gas Flows to Stabilize	When the Wait for Gas Flows to Stabilize check box is selected, the instrument remains in Preparing for Run state until the following ion source gas pressures have stabilized depending on the used ion source: • Sheath Gas (Arb) • Aux Gas (Arb) • Sweep Gas (Arb) When the ion source gases have reached the values defined in the instrument method, data acquisition starts.
Wait for Temperatures to Stabilize	When the Wait for Temperature to Stabilize check box is selected, the instrument remains in Preparing for Run state until the following ion source temperatures have stabilized depending on the used ion source: • Ions Transfer Tube Temp (°C) • Vaporizer Temp (°C) When the ion source temperatures have reached the values defined in the instrument method, the data acquisition starts.
Ion Source	
Default Source	• NSI (optional) • Heated ESI (H-ESI) • APCI (atmospheric pressure chemical ionization) (optional) • ESI **Note** Although atmospheric pressure photoionization (APPI) is not a configuration option, the mass spectrometer automatically detects if the ion source contains the APPI vacuum ultraviolet (VUV) lamp through the lamp's USB connection.
Default Source Type	Default Source Type: Heated ESI or APCI • Dedicated Heated ESI or Dedicated APCI • Combination Source

Parameter	Description
Enable Sweep Gas for NSI Source	Provides sweep gas flow to the NSI source.
	IMPORTANT Sweep gas can aid in the desolvation of the nanospray, but excessive sweep gas can deflect the nanospray from the orifice of the ion transfer tube, which decreases sensitivity. You must have the ion sweep cone installed for the sweep gas to work.
Enable Minimum Gas Flow Requirement for Sealed Sources (H-ESI, ESI, APCI, and APPI)	Provides minimum background flow of ion source gases to keep the source housing pressurized.
	IMPORTANT A minimum flow of gas compensates for the suction of the transfer capillary. This keeps the spectrum background clean by reducing the backflow of fumes from the drain tube/waste bottle. By default, the auxiliary gas will be forced to stay non-zero.
Optional Hardware	
Internal Calibration (EASY-IC) Source	Switches on/off the EASY-IC™ ion source.
Analog Inputs	
Channel 1 in Use	Reads the 0–10 Vdc analog input signal from an external device and writes the data into the raw data file. For additional information, refer to the instrument manual.
Channel 1 Label	The name you provide for channel 1.
Channel 2 in Use	Reads the 0–10 Vdc analog input signal from an external device and writes the data into the raw data file. For additional information, refer to the instrument manual.
Channel 2 Label	The name you provide for channel 2.
Buttons	
OK	Saves the instrument configuration settings and closes the window.
Cancel	Closes the Instrument Configuration window without saving your changes.
Apply	Applies the changes you made in the Instrument Configuration window.

3

Tune Application

This chapter describes how to use the Tune application to control, monitor, tune, and calibrate the Thermo Scientific™ Orbitrap Exploris Series mass spectrometer (MS). You can also optimize the instrument for your specific compounds, perform method development, and run real-time mass spectrometry experiments one analysis at a time.

Contents

Overview of the Tune Application

Use the Tune application to operate the Orbitrap Exploris Series MS with the data system computer. The Tune application organizes its functions in panes and on pages. To display the panes and pages, click the associated buttons and tabs.

The Tune application has the following main components:

- Three system power icons to set the MS's power mode (on, standby, and off).
- The system readback icon to indicate the various readback states.
- Three panes on the left to define parameters for scanning, ion source, and calibration.
- Four panes on the right to display information about instrument status, history and favorite settings.
- Up to three graphs to show real-time information about the current measurement.

❖ **To display the Tune application**

Choose **Start > All Programs > Thermo Instruments > Orbitrap Exploris Tune**.

Tip You can set a few preferences for how the Tune application works. Click the **Options** icon,  , and then choose **Preferences**.

Buttons and Icons

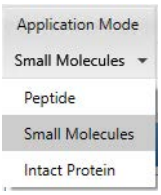
For complete descriptions of features, see the applicable table of the Tune icons and buttons.

System Power Icons

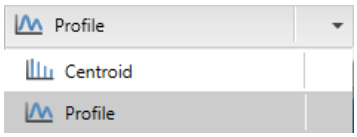
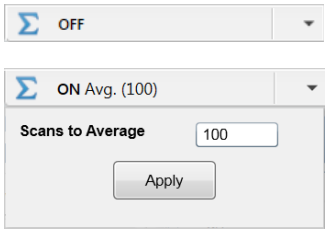
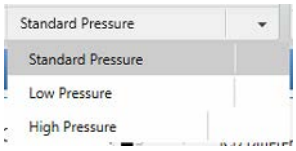
Button	Description
A green button indicates the active instrument status.	
On mode 	In the On state, all voltages, the sheath gas, the auxiliary gas, and the sweep gas are on.

Button	Description
Standby mode 	In the Standby state, the high voltages and the vaporizer heater are off. The RF voltages and the DC offset voltages remain on. The sheath gas and the auxiliary gas remain on at a low flow rate (6 arbitrary units).
Off mode 	In the Off state, the RF and high voltages, ion transfer tube heater, and vaporizer heater are off. In addition, the offset voltages are off. The sheath gas, auxiliary gas, and ion sweep gas remain on at a low flow rate to flush vapors from the ion source.

Application Mode

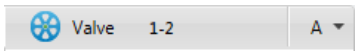
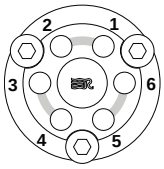
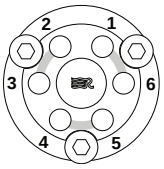
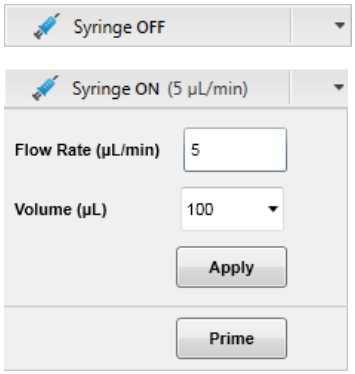
Button	Description
	See the menu item descriptions below.
Peptide	This application mode provides default instrument settings for the analysis of complex peptide mixtures.
Small Molecules	This application mode optimizes instrument settings for the analysis of small molecules with focus on quantification.
Intact Protein	This application mode optimizes instrument settings for the analysis of large molecules such as Intact Proteins, monoclonal Antibodies, and other macromolecules. You can use the pressure mode settings for optimized analysis of intact proteins under denatured or native conditions.
	Note This option is available only when the BioPharma license is installed.

Instrument and Spectrum Buttons

Button	Description
	Indicates the ion polarity mode (positive or negative).
	Indicates the data type mode (centroid or profile).
	Indicates whether the spectrum scan averaging is off or on and has the number of scans to average. Range: 2–1000 **Note** The Tune application displays the averaged spectrum in a brown color. The spectrum header displays the number of averaged scans in the scan filter (for example, AV:2).
	Indicates the mass spectrometer pressure mode. Available options are: • Standard Pressure: Optimal detection for intact protein mass and top-down detection of large fragment ions. • Low Pressure: Optimal detection for small molecules, bottom-up and top-down protein experiments. • High Pressure: Optimal detection for native protein analysis experiments. **Note** This feature is available only when the BioPharma license is installed.

Modular Valve and Syringe Pump Buttons

The Tune application displays these buttons for H-ESI, APCI, APPI, and NSI modes.

Button	Description
	Indicates the position (1-2 or 1-6) for two divert/inject valves (A and B) on the button left side. The down arrow opens two choices: valve A and optional valve B.  Position 1–2  Position 1–6
	Indicates whether the syringe pump is pumping. The syringe pump settings box defines the pump flow rate and the syringe volume. You can also prime the syringe by pressing and holding Prime. Syringe pump flow rate (µL/min): 0.05–500 Syringe volumes: 50, 100, 250, 500, 1000, and 10 000 Syringe priming (µL/min): 100

Data Acquisition Buttons

The Tune application saves the acquired data to a raw data file (.raw extension).

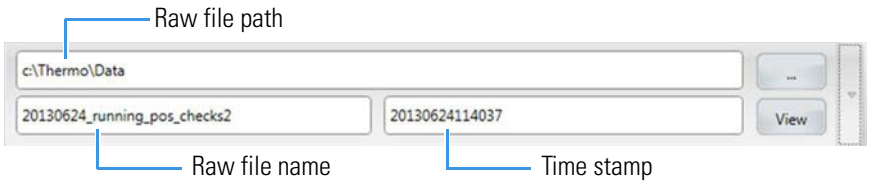
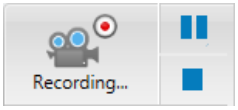
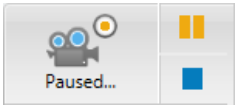
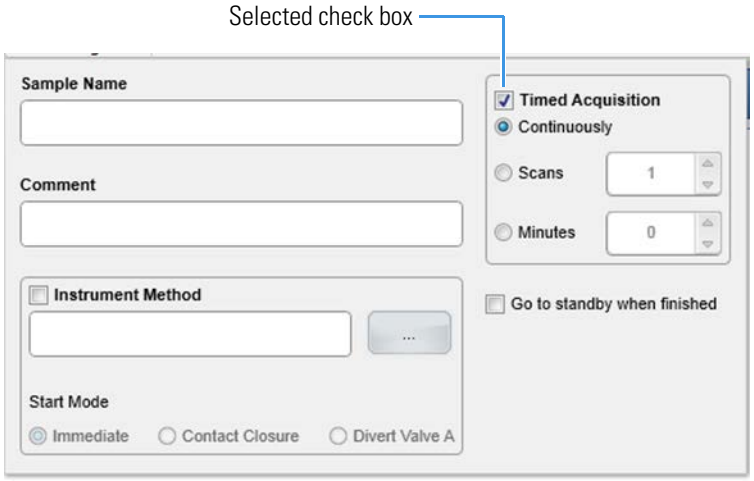


Figure 3-1. Raw file data

Button	Description
Note Click the label below the Record button to expand the acquisition settings box.	
Recording off  Recording on  Recording paused 	Click the **Record** toggle button to acquire data to a new raw data file. The name of the file—if not changed—is a combination of the base file name and a time stamp, which consists of the year (*YYYY*), month (*MM*), day (*DD*), and time (*HHMMSS*). To stop the data acquisition, click **Stop** (blue square). The color of the square then changes to green. To pause the data acquisition, click **Pause** (two blue bars). The color of the bars then changes to orange. To resume the data acquisition, click **Paused** (shown as an orange circle). **Note** If the Instrument Method check box in the data acquisition settings box is selected, the Pause feature is not available.
	(Optional) To change the destination folder for the raw data, click the Browse button. The default folder location is in drive:\Thermo\Data.
	You must manually set FreeStyle as the default application to view the RAW files. (To specify the default application, right-click the RAW file, then navigate to ThermoFisher.FreeStyle.App.exe (C:\Program Files (x86)\Thermo\FreeStyle).
Sample information and data acquisition method	
	Click the button to the left of the View button to expand the acquisition settings box. As shown in this figure, you can select only one check box. 
Sample Name	The name of the sample.
Comment	A comment that describes the acquisition.

Button	Description
Instrument Method	Indicates to load an instrument method and start the data acquisition with one of these options: • Immediate: Starts the acquisition immediately when you click **Record**. • Contact Closure: Starts the acquisition when the mass spectrometer receives a contact closure signal from the connected analog autosampler. • Divert Valve: Starts the acquisition when the position of the divert/inject valve changes from its current position.
Timed Acquisition	Indicates how long the mass spectrometer acquires data as follows: • Continuously: The mass spectrometer acquires data until you click **Stop**. • Scans: The number of scans acquired by the mass spectrometer before the data acquisition stops. • Minutes: The time (in minutes) that the mass spectrometer acquires data.
Go to Standby When Finished	The mass spectrometer goes in standby mode when the current acquisition is completed.
Enable FAIMS CV Scan	This parameter is available only when the system has detected an FAIMS source. Indicates the use and configuration of the FAIMS compensation voltage (CV) scan tool. The Start and Stop values defining the FAIMS CV range. The Step value defines the step size in volts within the range. The Estimated Duration read-only value counts down the estimated completion time (in seconds) for the CV scan. Range (start/stop): –300 to 300; default: –100 to 100 Range (step): 0.1–2; default: 1

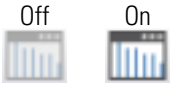
Instrument Status Icons

Icon	Description
Note When you start data acquisition, the instrument status icon does not change.	
Normal 	The system parameters are within tolerance.
Initializing 	The system is initializing.

Icon	Description
Changing Settings 	One or more settings are changing.
Source Off 	The ion source is off.
Disconnected 	There is no communication between the mass spectrometer and the data system.
Error 	An error has occurred.

Miscellaneous Icons

Icon	Description
This icon appears at the far right side of the Tune window, below the Instrument Status icon.	
	Displays the Options menu.
These icons appear at the bottom of the Tune window.	
Copy 	(Ion Source page) Copies the ion source parameters to the clipboard.
Paste 	(Ion Source page) Pastes the ion source parameters from the clipboard. **Tip** You can use the clipboard to transfer the ion source parameters between the Tune application and the Method Editor application.
Diagnostics 	Displays the Diagnostics pane.

Icon	Description
Monitor Mass Accuracy 	Displays the Monitor Mass Accuracy dialog box. Plots the difference between the measured peak position and the theoretical peak positions in the mass list. To start or stop monitoring the mass accuracy, click the icon.
Plot Chromatogram 	Displays the Plot Chromatogram dialog box. Plots a chromatogram for the TIC, Base Peak, or User Defined *m/z*. Additionally, the Spray Stability as %RSD of the ion current can be plotted. The %RSD must be less than 15% for the spray stability to pass the evaluation in the beginning of a calibration procedure. To start or stop the ion current display, click the icon.
Rotate Plots 	Permutates the displayed graphics.
Graph mode 	Divides the screen into up to three areas.

Displaying Real-Time Chromatograms and Spectra

See these topics and the button descriptions in Miscellaneous Icons:

- Controlling the Chromatogram View
- Monitoring the Mass Accuracy and Signal Stability
- Zooming In on a Spectrum
- Header Information in the Spectrum View
- Buttons and Icons

Controlling the Chromatogram View

Use the Plot Chromatogram dialog box to plot the chromatogram from the TIC, the base peak, or one or more user-defined *m/z* values. For the user-defined mass table, you can import the settings from (or export them to) a CSV, a TXT, or an XML file.

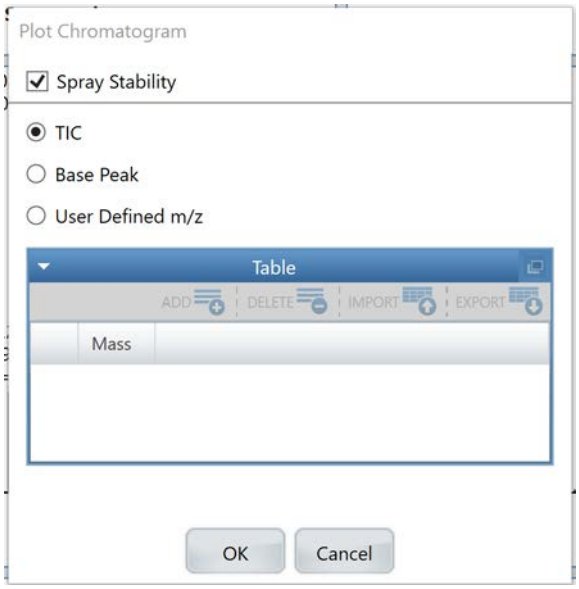


Figure 3-2. Plot Chromatogram dialog box

Note The Tune application always displays the Chromatogram view. Observe the chromatogram trace to see how system parameter changes affect the ion signal intensity so that you can optimize the parameter settings as needed.

❖ **To display the TIC or the ion current for a select mass as a function of time**

1. Click the **Plot Chromatogram** icon,  , at the bottom of the Tune window.

2. Select the chromatogram type, and then click **OK**.
3. Chromatogram data and spray stability data (if selected) are shown in separate windows during the monitoring.
4. To stop the plot, click the Plot Chromatogram icon again.

Parameters in the Plot Chromatogram Dialog Box

Parameter	Description
Spray Stability	Plots the spray stability. Plots a chromatogram for the TIC/Base Peak or User Defined *m/z*. Additionally, the Spray Stability as %RSD of the ion current can be plotted. The %RSD must be less than 15% for the spray stability to pass the evaluation in the beginning of a calibration procedure.
TIC	Plots the TIC chromatogram.
Base Peak	Plots the base peak chromatogram.
User Defined *m/z*	Plots the signal intensities of the ions you enter in the mass table as a function of time.
Mass table	
Mass	(User Defined *m/z*) Indicates up to 10 *m/z* values for the ion signal intensities that you want to plot. Range: 40–3000 (40–8000 with BioPharma option), default: 195.0877

Monitoring the Mass Accuracy and Signal Stability

Use the Monitor Mass Accuracy dialog box to plot the difference between the measured and theoretical peak positions in the mass list. For the mass table, you can import the settings for the mass table from (or export them to) a CSV, a TXT, or an XML file.

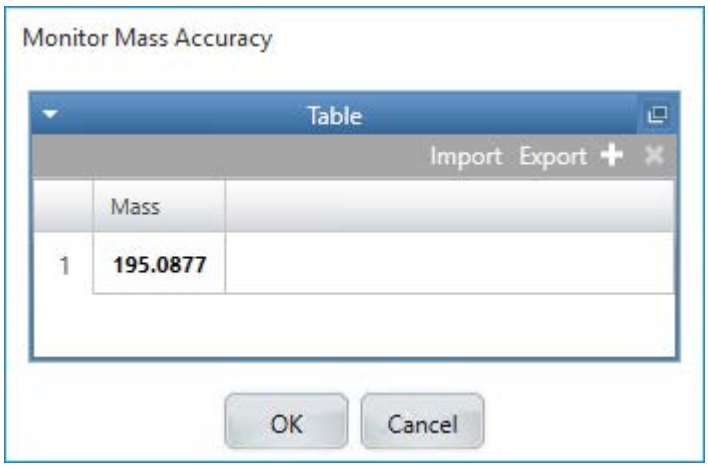


Figure 3-3. Monitor Mass Accuracy dialog box

❖ **To monitor the mass accuracy and signal stability**

1. Click the **Monitor Mass Accuracy** icon, , at the bottom of the Tune window.
2. Enter one or more *m/z* values with up to four decimal places accuracy within the allowed scan range. Then click **OK**.

   Note When you enter masses in the table, include at least two decimal places.

3. A plot "Monitoring Mass Accuracy" starts in the upper view panel: mass list entries are identified within a mass tolerance of ±25 ppm. Mass accuracy (ppm) is plotted against the scan number. The monitored mass traces are shown in the legend of the plot.
4. To stop the plot, click the Monitor Mass Accuracy icon again.

Parameters in the Monitor Mass Accuracy Dialog Box

Parameter	Description
Mass	Indicates up to 10 *m/z* values for the peaks that you want to monitor in the mass list. Range: 40–3000 (40–8000 with BioPharma option); default: 195.0877
Buttons	
OK	Displays the mass accuracy plot. To stop monitoring the mass accuracy, click the icon.
Cancel	Closes the dialog box without saving the entered data.

Zooming In on a Spectrum

In the Spectrum view, you can zoom in on one or both axes as needed.

❖ **To zoom in on a spectrum**

- To zoom in on both axes, drag the cursor diagonally across the spectrum to make a rectangle where the corners define the displayed axes ranges.
- To zoom in on one axis, drag the cursor horizontally or vertically along the axis or the spectrum to define the displayed range.

To go back to the default view, choose **Reset Scaling** in the shortcut menu.

Shortcut Menu Commands in the Spectrum View

Command	Description
Reset Scaling	Resets the axes to the default intensity and mass ranges.
Copy to Clipboard	Copies a screen capture of the mass spectrum to the Clipboard.
Pan	To use this tool, you must first zoom in on the spectrum. Then you can select this tool to slide the spectrum back and forth along the *x* axis by holding down the left mouse button and moving the mouse cursor.
Print	Sends a copy of the mass spectrum to the printer.
Show Frequency	Displays the frequency spectrum (in kHz) in blue. Clear this option to display the *m/z* spectrum.
Show Absolutes	Changes the *y*-axis scale from percentages to ion flux (ions/s).
Display	• Normalized: The *y*-axis scale of the mass spectrum normalizes so that the most intense peak equals 100. • Fixed: The *y*-axis scale of the mass spectrum does not change. • Creep: The *y*-axis scale of the mass spectrum automatically increases if the peak intensity increases, but does not decrease if the peak intensity decreases.

Command	Description
Profile Label	Adds the resolution (R) and charge state (z) values next to the peak labels.
Profile Label Setting	• Resolution: Calculates the resolution (R) and labels the peaks with it. • Charge: Labels the peaks with the charge state (z).

Header Information in the Spectrum View

This table defines the information at the top of the real-time spectrum.

Header information	Description
Scan number (#)	The scan count, which only resets to zero when you start data acquisition.
RT	The retention time (in minutes), which also resets to zero when you start the data acquisition.
NL	The normalization level, which is a measure of the ion signal intensity.
Injection time	The injection time (in milliseconds) per scan.
Scan settings (filter)	The detector type, polarity mode (+ or –), data type (profile or centroid), source type, scan type, and other settings.

Controlling the Ion Source

The Ion Source pane uses the following real-time indicators to identify the readback status for each parameter:

- Green square ( )—Indicates that the parameter has reached the specified value.
- Orange square ( )—Indicates that the parameter is trending toward the specified value.
- Red square ( )—Indicates that the parameter could not reach the specified value.

Note A red border around a parameter box indicates that the value is out of range.

Tip After setting the parameters on the Ion Source pane, you can use the button to copy the parameters settings for pasting into an instrument method.

Parameters on the Ion Source - Ion Source Page

Use the Ion Source pane to set the ion source parameters.

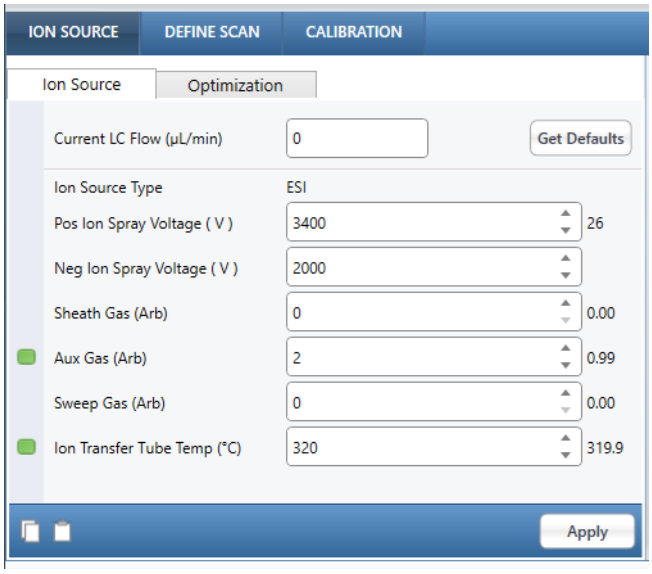


Figure 3-4. Tune application—Ion Source page

Parameters for the H-ESI, APCI, and NSI Ion Source Types

Parameter	Description
Current LC Flow (µL/min)	(Ion Source Type: H-ESI or APCI) The LC flow rate (µL/min). Click **Get Defaults**, and then click **Apply** to update the ion source parameters. The Tune application sets the applicable ion source parameters to the appropriate default values for the specified LC flow rate. Range: 0–3000; default: 0
	Note • Clicking Apply does not start the LC. • When the ion source is in off mode or standby mode, it is pressurized with background nitrogen gas to avoid back-streaming from the drain and introducing contaminants.
Ion Source Type	The configuration for the ion source housing. The instrument automatically recognizes the source type and displays the corresponding parameters for the detected source type. In case of a combo ion source (Heated ESI and APCI), you can select the source type that you want to use.
	Note Although atmospheric pressure photoionization (APPI) is not a configuration option, the mass spectrometer automatically detects if the ion source contains the APPI vacuum ultraviolet (VUV) lamp through the lamp's USB connection.
Pos Ion Spray Voltage (V) Neg Ion Spray Voltage (V)	(Ion Source Type: H-ESI or NSI) The source spray voltage (absolute value, in volts). Positive polarity range: 0–6000 (H-ESI) or 0–3000 (NSI); default: 3400 (H-ESI) or 1500 (NSI) Negative polarity range: 0–5500 (H-ESI) or 0–2500 (NSI); default: 2000 (H-ESI) or 1500 (NSI)
Sheath Gas (Arb)	(Ion Source Type: H-ESI or APCI) The sheath gas flow rate (arbitrary units). Range: 0–80; default: 0 (or determined by the Tune application based on the LC flow rate)

Parameter	Description
Aux Gas (Arb)	(Ion Source Type: H-ESI or APCI) The auxiliary gas flow rate (arbitrary units). Range: 0–25; default: 2 (or determined by the Tune application based on the LC flow rate) **Note** If the vaporizer temperature is set to values above 100 °C, the auxiliary gas is automatically set to 5 unless it is set higher manually.
Sweep Gas (Arb)	The sweep gas flow rate. Range: 0–20; default: 0 (or determined by the Tune application based on the LC flow rate) **Note** In the Instrument Configuration, you can switch on the sweep gas for the NSI source.
Ion Transfer Tube Temp (°C)	The temperature of the ion transfer tube (degree Celsius). Range: 0–400; default: 320 (or determined by the Tune application based on the LC flow rate)
Vaporizer Temp (°C)	(Ion Source Type: H-ESI or APCI) The temperature (degrees Celsius) of the APCI vaporizer, which vaporizes sample and solvent, or of the H-ESI source heater, which heats the auxiliary gas. Range: 0–550; default: 0 (off) (or determined by the Tune application based on the LC flow rate) **Note** You must set the auxiliary gas to 5 or greater for vaporizer temperatures above 100 °C.
Pos Ion Discharge Current (µA) Neg Ion Discharge Current (µA)	(Ion Source Type: APCI) The APCI source discharge current (microamperes). Range: 0–100; default: 4 (positive polarity mode) and 10 (negative polarity mode) **IMPORTANT** The actual possible maximum value of the discharge current is limited by the maximum value of the spray voltage of 5000 V.

Parameter	Description
APPI Lamp	(Ion Source Type: H-ESI or APCI) Switches on or off the optional APPI lamp. Tune displays the readback value for the current lamp state next to the list box, where 0 is off and 1 is on. Default: Off **Note** The Tune application displays this parameter only when the ion source contains the optional APPI lamp. The lamp state shown in the application might not match the lamp state shown in Method Editor if an instrument method uses APPI mode.

Parameters for the FAIMS Pro System

For additional information, refer to the *FAIMS Pro System User Guide.*

Parameter	Description
Total Carrier Gas Flow (L/min)	The flow rate for the FAIMS and carrier nitrogen gas. Range: 0.7–4.3; default: 1.2
FAIMS Mode	The temperatures for the FAIMS electrodes are as follows: • Standard Resolution: Provides the best transmission mode by setting the inner and outer electrodes to 100 °C. • High Resolution: Provides twice the resolution of the standard resolution mode by setting the inner electrode to 80 °C and the outer electrode to 100 °C. • User Defined: Displays the fields to enter the electrode temperatures. **Note** The electrode temperatures affect ion separation. Although ion transmission might be lower in FAIMS high resolution mode, the peaks are narrower due to the electrodes' temperature differential.
FAIMS Inner Electrode Temp (°C)	(FAIMS Mode: User defined) The maximum temperature for the inner electrode in the FAIMS Pro system. Range: 70–100; default: 100
FAIMS Outer Electrode Temp (°C)	(FAIMS Mode: User defined) The maximum temperature for the outer electrode in the FAIMS Pro system. Range: 70–100; default: 100

Optimizing the Ion Source Parameters

Follow this procedure for the H-ESI and APCI source types to maximize the ion signal for your application.

Note A red border around a parameter box indicates that the value is out of range.

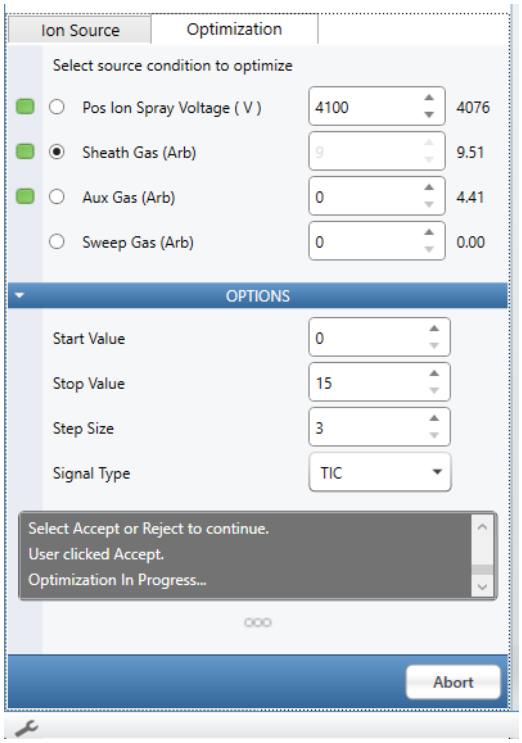


Figure 3-5. Tune application—Optimization page

During the optimization, the Tune application displays the progress. While the optimization procedure is running, the upper right graph window plots Intensity RSD values per optimizing condition (10 scans).

After the optimization procedure is finished, the upper left graph window displays a smoothed optimization curve, the optimized parameter value in the legend box, and highlights this value with a vertical line in the graph.

You can abort the optimization. When the optimization completes, you can choose to generate a report. Then, an Ion Source Optimization Report is generated and presented to you.

❖ **To optimize the ion source parameters**

1. On the Ion Source - Optimization page, select the parameter that you want to optimize (for example, start value, stop value, step size, and signal type options).

2. To enter the value of a parameter, click the arrow in the spin box to increase [up arrow] or to decrease [down arrow] the value. Or, enter the value in the spin box text field.
3. If applicable, select the required option in the list box.
4. Click **Optimize.**

Parameters for the Ion Source - Optimization Page

Parameter	Description
Spray Voltage (V)	(H-ESI mode) Optimizes the source electrospray voltage (absolute value, in volts).
Sheath Gas (Arbitrary)	(H-ESI and APCI modes) Optimizes the sheath gas flow rate (in arbitrary units).
Aux Gas (Arbitrary)	(H-ESI and APCI modes) Optimizes the auxiliary gas flow rate (in arbitrary units).
Sweep Gas (Arbitrary)	Optimizes the sweep gas flow rate (in arbitrary units).
Discharge Current (μA)	(APCI mode) Optimizes the APCI source discharge current (in microamperes).
Options	
Start Value	The initial value of the parameter being optimized.
Stop Value	The final value of the parameter being optimized.
Step Size	The step size of the parameter being optimized.
Signal Type	• TIC (default): Maximizes the total ion current (TIC) signal. • Base Peak: Maximizes the base peak signal. • *m/z*: Maximizes the signal of the ion with the *m/z* value that you specify in the *m/z* box.
m/z	(Signal Type: *m/z*) The *m/z* of the ion to optimize on.
Buttons	
Optimize	Starts the optimization based on the ion source parameters.
Abort	Stops the optimization based on the ion source parameters.
Accept	Accepts the optimized ion source parameter.
Reject	Rejects the optimized ion source parameter.

Setting Up the Mass Spectrometer for Data Acquisition

Set up the mass spectrometer for data acquisition by using the Define Scan pane. For the mass table, you can import the settings from (or export them to) a CSV, TXT, or XML file.

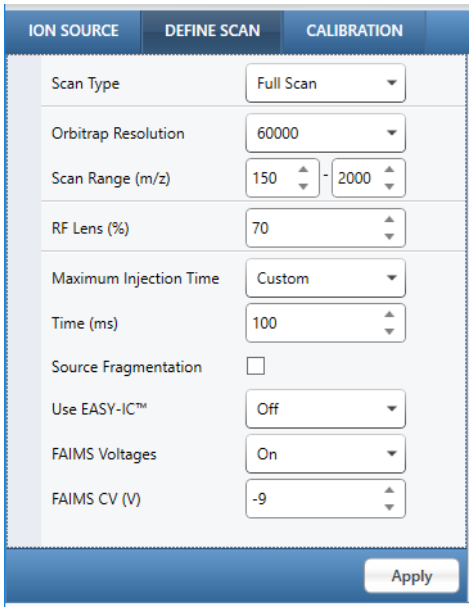


Figure 3-6. Tune application—Define Scan pane (Full Scan)

Specifying the Scan Settings

❖ **To specify the scan settings**

Select from the following parameters.

Parameter	Description
Scan Type	• Full Scan: One stage of mass analysis. • EASY-IC™ Calibrant: Displays the reagent ion spectrum for *m/z* 202 for the internal EASY-IC™ ion source.
	IMPORTANT When you select EASY-IC™ Calibrant, the isolation width and all other *m/z* scan parameters are automatically set to allow for the detection of the fluoranthene reference mass.

Parameter	Description
Orbitrap Resolution	The mass resolution of the Orbitrap analyzer, which is proportional to the inverse square root of the mass-to-charge ratio. Mass resolution is defined as the observed *m/z* value divided by the smallest difference Δ *m/z* for two ions that can be separated: *m/z* / Δ *m/z*. Spectra acquired at higher Orbitrap Resolution allow greater resolution in *m/z* but take longer to acquire. The selected resolution is specified for a peak at *m/z* 200. The available options are: 15 000, 30 000, 60 000, 120 000 (default), and 180 000.
Scan Range (m/z)	The values for the Scan Range (*m/z*). Range: 40–3000 (40–8000 with BioPharma option); default: 200–3000
RF Lens (%)	Specify the value to control the RF amplitude applied to the S-lens. Range: 0–200; default: 70 This value is a scaling factor applied to the nominal mass-to-voltage relationship. Decreasing the RF level decreases the transmission of high *m/z* ions through the S-lens, increases the transmission of the low *m/z* ions, and might decrease the amount of fragmentation of fragile ions in the S-lens. Increasing the RF level has the opposite effects. **Tip** For stable ions, the default value provides a good starting point. A fine tuning of the MS is recommended, however.
AGC Target	Indicates Standard (default) or Custom for the Automatic Gain Control™ (AGC) target value, which controls the number of ions that are injected into the mass analyzer. • Standard: The system sets the recommended target in an automated fashion per scan type and user-defined settings (default). • Custom: You set the AGC Target based on the Standard AGC Target.

Parameter	Description
Normalized AGC Target (%)	(AGC Target: Custom) Specifies the Automatic Gain Control (AGC) target. This is a percentage representing the maximum number of charges to accumulate for a given analysis. Range: 1–1000; default: 100 This is the normalized AGC Target value, it is represented as a percentage to aid in calculating the desired AGC Target. The base normalized value is different for scan types. The values are as follows: Scan Type = Full Scan; Normalized Base (100%) = 1e6 The IRM collects ions until it reaches the AGC Target or the maximum injection time. The MS then transfers the ions to the Orbitrap analyzer.
Maximum Injection Time	Specifies the maximum injection time (max IT) that is allowed to reach the AGC Target. The IRM collects ions until it reaches the AGC Target or the max IT. The mass spectrometer then transfers the ions to the Orbitrap analyzer. • Auto: The system calculates the maximum injection time available (according to the transient length) to balance between sensitivity and scan speed (in parallel acquisition). • Custom: You can define the maximum injection time for the scan type. When using “Custom,” you can extend the max IT beyond the transient length of the Orbitrap scan. Please be aware that the instrument may slow down if the total max IT is utilized. When extending the max IT to double the transient length (for example, 55 ms for 15k resolution), you should consider using a higher resolution (in this example 30k) because this also improves the S/N by a factor of ca. 1.4. In targeted (quantitative) experiments, longer injection times (when allowed by longer max ITs) may lead to higher sensitivity.
Maximum Injection Time (ms)	(Maximum Injection Time: Custom) Maximum time that is allowed to accumulate ions in the IRM until the AGC Target is reached. Range: 1–1000; default: 100

Parameter	Description
Microscans	Number of scans to average in a given spectrum. Range: 1–10; default: 1 A microscan is one ion injection followed by ion detection. The MS sums microscans to produce one scan, which improves the signal-to-noise ratio of the mass spectral data. **Note** The overall scan time increases linearly with the number of microscans, significantly slowing the rate of spectral acquisition.
Source Fragmentation	Select the check box to switch on ion source CID. An offset voltage in the ion source accelerates the ions into background gas. Collisions with the background gas might aid in the desolvation of the ions and might increase sensitivity.
Energy (V)	(Source Fragmentation: On) Specifies the collision energy voltage for ion source fragmentation. Range: 1–135; default: 35 If you set the source fragmentation energy too high, fragmentation of ions may occur.
Use EASY-IC™	(Internal Mass Correction: EASY-IC™) Provides an internal reference mass, which is used for mass correction during a run.
FAIMS Voltages	Switches On (default) or Off the FAIMS voltages.
FAIMS CV (V)	(FAIMS Voltages: On) The optimized FAIMS compensation voltage. Range: –300 to 300; default 0 For the purpose of harmonization between platforms, the observed CV values on Orbitrap Exploris Series instruments were aligned with those of the Tribrid and TSQ platforms. This means the transmission for one *m/z* should be the same for the same CV setting on all three platforms. For targeted CV experiments, it is recommended to use the value that was determined by a CV scan (performed in the Tune window) or optimized with single CV experiments within an HPLC run.

Acquiring a Data File with the Tune Application

❖ **To acquire a sample data file**

1. Open the Data Acquisition pane, and then do the following:

a. (Optional) To change the destination folder for the raw data, click the  button.

   The default folder location is in C:\Thermo\Data.

b. In the File Name box, type the name of the analyte (for example, reserpine).

   If the base file name already exists in the save location, the Tune application adds a time-stamp suffix that consists of the year (*YYYY*), month (*MM*), day (*DD*), and time (*HHMMSS*).

c. In the Sample Name box, type the name of the analyte (or another suitable label).

d. In the Comment box, type a comment about the experiment.

   For example, describe the ionization mode, scan type, scan rate, sample amount, or method of sample introduction. The data system includes the comment in the header information for the raw data file.

e. Under Timed Acquisition, select the **Continuously** option (acquires data until you stop the acquisition).

2. Click **Record** to start data acquisition.

   After the Tune parameters reach their specified settings, the data acquisition process begins and the small circle on the Record button changes to red ().

   When you are finished, click **Record** again to stop the acquisition.

The small circle on the Record button changes to gray (not recording).

Tuning, Calibrating, or Checking the Mass Spectrometer Calibration

You can tune, calibrate, or check the mass spectrometer calibration with the special calibrant probe (Ion Source Type: ESI).

Use the FlexMix™ calibration solution (Pierce™ P/N A39239) to calibrate the Exploris Series instrument:

- It is designed for both positive and negative mass calibration in the range from *m/z* 40–3000.
- Store it at room temperature. Do not expose it to light or heat.

IMPORTANT After a bakeout, the system must be re-calibrated. The instrument recognizes that it has been vented and adds certain calibration steps to the system calibration that only need to be run after a bakeout.

Note

- You can set a few preferences for how the Tune application works. Click the **Options** icon,  , and then choose **Preferences**.
- If a System Calibration fails, restarting the calibration applies the values from the previously successful sequence and continues from that previous point.

Calibration Procedures

The Calibration pane shows the last time you calibrated the mass spectrometer. Generally, you should calibrate the mass spectrometer every month of operation for optimum performance over the entire mass range.

Note We recommend to use the calibrant probe (Ion Source Type: ESI) for all calibrations. In the course of the ion source optimization, monitor the Spray Current in the Status pane (Ion Source > Spray Current). Make sure that the Spray Current is not higher than 0.5 µA in positive mode and not higher than 0.3 µA in negative mode.

IMPORTANT While running the calibration procedures, you cannot run methods in the Xcalibur data system.

Calibration parameters are instrument parameters that affect the efficiency, sensitivity, mass accuracy, and resolution of the ion accumulation and detection process.

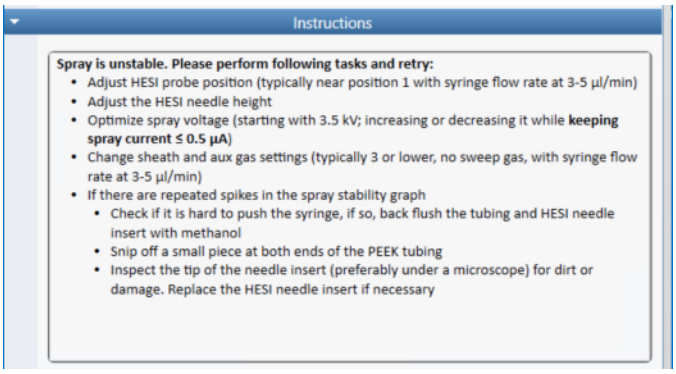
Tune parameters are instrument parameters that affect the magnitude of the ion signal. There are two types of tune parameters:

- Mass-dependent—Affects the RF voltage of the S-lens and the DC offset voltages of the lenses and multipoles. Use the Calibration Options pane to optimize the mass-dependent tune parameters.
- Compound-dependent—Affects the ion source parameters, such as the spray voltage or spray current, and the sheath, auxiliary, and sweep gas flow rates. See Optimizing the Ion Source Parameters to optimize the compound-dependent tune parameters.

The Calibration pane has the following parameters:

Parameter	Description
Status	
Polarity	Select the polarity for which you want to see the calibration data.
Recommended Calibrations	This is the recommended date for recalibration. The recommendations are based on the dates of the last successful calibrations and predetermined time intervals. Dates displayed in bold and italic font indicate that the recommended date has been exceeded. If the calibration failed, the recommended date is the current date.
Last Successful Calibration	This is the date of the last successful calibration.
Calibration	
During the calibration, the Tune application displays event messages in the gray window: • Started/finished subprocedures with results • Reached/resumed checkpoints • Calibration result The system reports all results in the gray window. The result is either “pass” or “failed.” If the result is “failed,” the system displays a recommended action based on the failure type.	
Mode	• Calibrate The system runs all selected mass calibration or system calibration procedures with selected polarity in the correct order. • Check The system runs all selected mass check or system check procedures with the selected polarity.
Polarity	Select the polarity for which you want to perform the calibration or check.

Parameter	Description
Type	• Mass: Uses the masses of a stable FlexMix spray to calibrate or check the mass accurracy. • Mass & System: Performs a whole system calibration or check. This calibration/check requires FlexMix solution. • One-Point Mass: Uses the internal calibration source with fluoranthene to calibrate the mass accuracies with one point. This calibration type can be performed anytime between runs without disconnecting the HPLC. You may subsequently evaluate the mass range for your analytes, for example with a system suitability test. **IMPORTANT** The one point mass calibration runs in both polarities—starting with the negative ion mode. • Customized Mass: Uses external masses from a list for the mass accuracy calibration. Click **Load user-defined mass lists** to get access to a directory where you can - recall/load available mass list files - save new mass list files - save updated mass list files - delete user-defined mass list files. To do so, delete the mass list file manually in the Windows Explorer. You can select provided mass lists and user-defined mass lists. A mass list can contain both positive and negative *m/z* values. **IMPORTANT** For each polarity, you can specify up to ten theoretical masses. The Tune application shows only the reference masses whose polarity matches the selected polarity. If you want to use a mass in a list, select the corresponding check box.

Parameter	Description
Instructions	
This field displays appropriate notifications about various routine states, for example spray stability, calibration mixture evaluation, contamination, or degradation. It gives recommendations about next steps to solve issues.  	

IMPORTANT To minimize the possibility of cross-contamination, do not use the same syringe and PEEK tubing for the calibration and the sample measurement. Before you start using your analyte, flush the inlet components again.

After the calibration, you see either a green check ( ) adjacent to the calibration name to indicate a successful calibration or a red X mark ( ) to indicate a failed calibration. A date appears in the Last Calibrated column for each successful calibration test. A date does not appear for failed calibrations.

Calibration Checkpoints

When a calibration fails, a regular report is generated. When you start the calibration again, all previous sub-procedures up to the checkpoint are replayed at a higher speed—including the graphs displayed.

A checkpoint becomes invalid:

- After 24 hours (after the calibration was initially started).
- On instrument reboot.

After four unsuccessful restarts of the calibration, all checkpoints become invalid and the calibration starts from the beginning.

After each calibration, you can choose to generate a report. A report generated after the finished calibration contains all successful parts of the entire calibration sequence, even those that came before the checkpoint.

IMPORTANT An unsuccessful or partially successful sequence does not change the instrument calibration. The calibration results are stored only when the whole system calibration has passed.

Using the Panes at the right Side

Four panes on the right of the Tune application window display information about instrument status, history and favorite settings. To expand or collapse the panes, click the  buttons.

Working with the Favorites Pane

The parameter panel of the Favorites pane shows the active ion source and several scan parameters.

The System Settings pane provides default Ion Source and Define Scan settings for the ESI Source recommended for calibrating the Orbitrap Exploris Series MS.

The User Settings pane allows you to save user-defined Ion Source and Define Scan settings.

Note You cannot rename or delete System Settings.

Saving a Favorite State

You can save the current key parameters of the mass spectrometer by using the Favorites pane. A validation procedure checks if the Ion Source settings and the Define Scan settings were applied before saving these parameters as Favorite settings. If this condition is not fulfilled, an error message appears that reminds you to apply the active settings.

❖ **To save a favorite state**

1. Modify parameters in one of the Ion Sources or Define Scan panes.
2. Click **Apply**.
3. Click the **Favorites** tab to display the Favorites pane.
4. In the Favorites pane, click **Save Current State**.
5. Type a unique name in the box that appears, and then click **Save Current State**.

   The newest favorite state appears first in the Favorites list. You may enter up to 100 states.

Loading a Favorite State

You can load the current or previously saved key mass spectrometer parameters by using the Favorites pane. When you *load* a favorite state, its key parameters appear in the Ion Source and Define Scan panes, but

the Tune application does not automatically submit them to the mass spectrometer. Changed properties are shown in bold in the parameter panel.

❖ **To load a favorite state**

Right-click the name in the Favorites list and choose **Load**.

The Tune application displays the key parameters in the Parameters box.

Applying a Favorite State

You can apply previously saved key mass spectrometer parameters by using the Favorites pane. When you *apply* a favorite state, the Tune application submits the parameters to the mass spectrometer and also displays them in the parameters panel.

❖ **To apply a favorite state**

Right-click the name in the Favorites list, and click **Apply** in the Ion Source or Define Scan pane.

Deleting a Favorite State

You can delete a saved favorites entry by using the Favorites pane.

❖ **To delete a favorite state**

Right-click the name in the Favorites list and choose **Delete**.

Renaming a Favorite State

You can rename a saved favorites entry by using the Favorites pane.

❖ **To rename a favorite state**

1. Right-click the name in the Favorites list and choose **Rename**.
2. Type a different name in the box that appears.

Viewing the Instrument Status

Use the Status pane and the Control pane to monitor the working condition of your instrument.

Using the Status Pane

The Status pane displays real-time status information in a tree view for many mass spectrometer parameters and components. The status readback indicators update every few seconds and are as follows:

- Green square ( )—Indicates that the parameter is within its expected range
- Orange square ( )—Indicates that the parameter is trending toward the expected range
- Red square ( )—Indicates that the parameter is outside of its expected range

❖ **To view the Status pane options**

1. Click the Status button at the right side of the Tune window.
2. In the header of the Status pane, click the downward arrow, and then choose **By Function** (default) or **By Board**.
3. Click the arrow next to the category that you want to expand.

Using the Control Pane

The Control pane displays real-time status information in a tree view for many mass spectrometer parameters and components. The status readback indicators update every few seconds and are as follows:


Info; status is normal / command successful


Warning; no user action required


Error; user action required


Fatal error; program cannot proceed

❖ **To view the Control pane**

1. Click the Control button at the right side of the Tune window.
2. Click the symbol next to the category that you want to expand.

Viewing the Tune History

The History pane records all parameter changes made in the Ion Source and Define Scan panes as “change records,” which appear as sub-items under the date they were created. A change record is inactive if the ion source type of the change record differs from the currently installed ion source type. The maximum number of change records is 100.

When you select a given time, the pane indicates what changes were made (shown in bold black) compared to current Ion Source settings and Define Scan Settings.

By right-clicking, you can either apply the settings directly or just load the settings into the parameter panel where you can then make further changes and apply them. By double-clicking on the change record, settings are directly applied into the parameter panel for further changes.

❖ **To view or modify a change record**

Choose from the following:

- Right-click a change record and choose **Load** to display its parameters. Parameters shown in bold differ from their default values.
- Right-click a change record and choose **Apply** in the Ion Source pane or Define Scan pane to submit its parameters to the mass spectrometer.

Generating Reports

You can generate a report after running the procedures on the Calibration and Diagnostics panes. Depending on the settings in the Tune Preferences dialog box, no report is created, the report is created automatically, or the Report Generation Options dialog box is displayed.

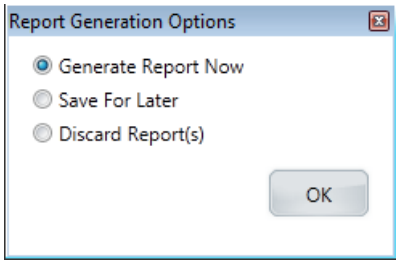


Figure 3-7. Report Generation Options dialog box

Select one of the following options:

- Generate Report Now: The PDF report is generated and saved in the following default folder: C:\Thermo\Instruments\Reports.
- Save For Later: You can specify a folder to save the PDF report to.
- Discard Report(s): No PDF report is saved.

The PDF report has the following content:

- The title distinguishes between Calibration Reports and Calibration Check Reports.
- The header contains Date & Time, Instrument Model name, Instrument Serial, and Software Version.
- The PDF report comprises a section header for every (sub-)calibration run.
- The table summarizes all calibration results or calibration check results:
  - The column “Name” includes name of Calibration; sub-steps are indented. A unit is shown where applicable.
  - The column “Result” comprises test result of a calibration/check shown as “Passed” highlighted in green or “Failed” highlighted in red. Sub-step results are shown as “Passed” or “Failed,” too.
  - The columns “Value”, Minimum” and “Maximum” are restricted to calibration/check values. If no relevant value is available, the field will be filled with “-”.

- The column “Comment” comprises further important information about passed results or reasons for failure.

- The mid section summarizes calibration/check plots and additional information for each Calibration/Check procedure; each procedure is highlighted in bold letters and a larger font.
- The PDF report is finalized by a general “System Configuration” report including graphs of some of the sub-procedures.

❖ **To generate a report**

1. In the Report Generation Options dialog box, select **Generate Report Now** and click **OK**.

   Note If you save the report for later, a Report button appears next to the Start button until you view the report. You cannot run methods in the Xcalibur data system until you view or cancel the saved report.

2. Save the report as a PDF file.

After completing the procedures, the Tune application prompts you to generate a report with the results.

Specifying Options for the Tune Application

The Options menu of the Tune application has the following commands:

Command	Description
Preferences	Displays the Tune Preferences dialog box.
Load standard diagnostics	Displays the Diagnostics pane (left pane).
View calibration reports	Gives access to the folder that contains the calibration reports.
View other reports	Gives access to the folder that contains other reports.
View Instrument	Displays a window that shows a schematic drawing of the instrument ion optics and analyzer.
Tune Help	Displays the Tune Help.
Instrument Manuals	Gives access to the folder that contains the instrument manuals that are installed with the Tune application.
Instrument Web page	Displays the website of the Orbitrap Exploris Series mass spectrometers.
About Tune	Displays the About dialog box with information about the instrument, the current Tune version, and the active licenses.

❖ **To display the Options menu**

Click the **Options** icon,  .

Setting Preferences for the Tune Application

Use the Tune Preferences dialog box to specify the behavior of the Tune application.

Figure 3-8. Tune Preferences dialog box

❖ **To display the Tune Preferences dialog box**

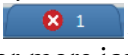
1. Click the **Options** icon,  .
2. Choose **Preferences**.

The Tune Preferences dialog box has the following parameters:

Parameter	Description
General	• Clear Calibration check boxes when complete • Clear Diagnostics check boxes when complete • Enable Hotlink for Define Scan and Ion Source Panel Select the Hotlink check box to allow the Tune application to send any changes immediately to the instrument.
Report Options	You can choose different options for calibration reports and other reports: • Automatically generate reports To change the destination folder for the reports, click the Browse button. The default folder location is in C:\Thermo\Instrument\Reports\. • Show Report Generation Options dialog box • Do not generate reports
Report Content Options	• Show Console • Show graph • Show spectrum • Show system configuration • Show embedded system configuration
Alerts Console Options	Use these parameters to specify what is displayed in the alerts console. • Show warnings • Show recovered errors and warnings • Show information • Minutes included in the log file before error detected • Minutes included in the log file after error detected

Parameter	Description
Mass Self-Calibration Options	Select **Run One-Point Mass Self-Calibration** to enable the periodic unattended calibration procedure. Use this procedure to ensure that the mass accuracy remains within the specifications for at least four weeks (when run daily). Use the parameters of the Schedule Self-Calibration area to specify the week days and the hours for the self-calibration. Whether the instrument actually performs the self calibration depends on its power mode: • Instrument in Standby: procedure runs • Instrument On without raw data acquisition: procedure runs • Instrument On with raw data acquisition: procedure remains on hold. If a sequence is active, the procedure runs when the sequence is finished. If multiple sequences (batches) are queued, the procedure runs between the active sequence and the next sequence in the queue. The next sequence will commence when the calibration has passed. • Instrument in Stop mode or Off: procedure is inactive The procedure generates a PDF report and stores the file on the data system computer. When the instrument passes the self-calibration, the system updates the master.cal file and the mass calibration performance status on the Calibration Status panel. **IMPORTANT** This parameter is available only when the Internal Calibration (EASY-IC) Source check box is selected in the Thermo Foundation Instrument Configuration window.

Using the Alerts Console

The alerts tab appears at the bottom of the screen only when the Tune application generates an alert message (for example,  , which indicates one [1] error). The application shows one or more icons that indicate the types of messages. You can filter the messages by type and sort their order by clicking any of the column headings.

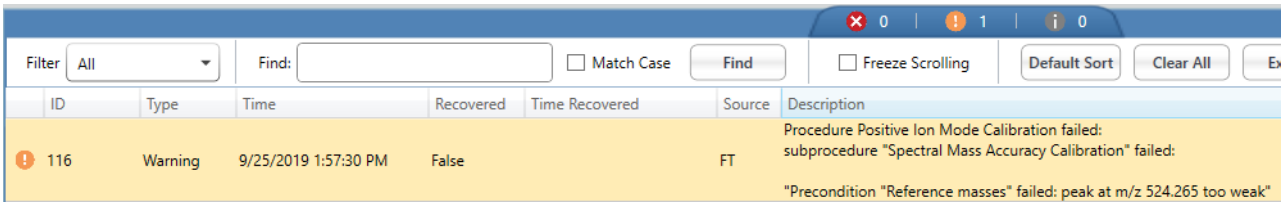


Figure 3-9. Alerts console

❖ **To open or close the alerts console**

When the alerts tab appears at the bottom of the screen, click it.

Parameters in the Alerts Console

Parameter	Description
Alert type icons	• Errors • Warnings • Recovered errors and warnings • Information The number after the icon indicates the total number of messages for this type.
Filter	Select the type of message to show.
Find	Searches the displayed messages by entering one or more keywords. To search all messages, set the Filter to All.
Match case	Makes the search case sensitive.
Freeze Scrolling	Prevents the list of messages from scrolling as new messages appear.
Buttons	
Default Sort	Resets the order of the alert types to show the errors first, then the warnings, and then the remaining messages sorted by time.
Clear All	Removes all of the messages, except for the active error and warning messages.
Export	Exports all alert messages to a CSV file.

About Dialog Box

Use the About dialog box to display information about the instrument, the current Tune version, and the active licenses. To copy the instrument identification to the clipboard, click the button.

The About dialog box has the following parameters:

Parameter	Description
End User License Agreement	Display various dialog boxes with legal information and information about third party licenses used by the Tune application.
Add license	Displays the License dialog box.
Close	Saves your changes and closes the dialog box.

❖ **To display this dialog box**

1. Click the **Options** icon, .
2. Choose **About Tune**.

Running Diagnostics

Only Thermo Fisher Scientific field service engineers can run the complete diagnostics on the mass spectrometer subsystems. As a customer, your access to the diagnostics is limited.

Tip You can set a few preferences for how the Tune application works. Click the **Options** icon,  , and then choose **Preferences**.

❖ **To perform diagnostics**

1. Click the **Diagnostics** icon,  , at the bottom of the Tune window.
2. Click the arrow next to the category that you want to expand.
3. Select the components that you want to test.
4. If necessary, enter new values for the selected parameters.
5. Click **Start**.

Category	Description
The descriptions for the individual parameters are built into the application. To see a tooltip description, point to the parameter name, and for additional information, click **Learn More**.	
System	A manual bake-out can be started, and various diagnostic checks can be performed. Also, you can evaluate the purity of the FlexMix calibration solution and burn in the internal calibration source.
Partial Calibration	When you know that certain subsystems might be out of specs, you can calibrate the healthy subsystems from here.
Optional Calibration	Procedures that provide additional calibrations to prepare the instrument for specific applications. For example, a dedicated low *m/z* mass calibration can be performed. It improves the mass accuracy for low *m/z* applications. However, the standard *m/z* mass accuracy (150–2000 *m/z*) may shift by a sub-ppm amount after running this procedure.
FAIMS	Contains procedures for the FAIMS source performance. The check boxes in this area are available only when the system has detected a FAIMS source.

Category	Description
Tools	Performs a soft reset, triggers MS processes, or switches on or off MS components.
Calibration > Skip Spray Stability Evaluation	This function allows to skip the spray stability check, which is run before the mass calibration. This allows to run the mass calibration with a less stable spray, for example when a mass calibration needs to be performed with the HESI sprayer. However, we strongly recommend the low-flow setup with the calibrant sprayer. Generally, the spray stability evaluation generates real-time graphs of the TIC and of the relative standard deviation (RSD) of the TIC. The %RSD must be less than 15% for the spray stability evaluation to pass. For the system calibration, the %RSD should be less than 10%. **Tip** If the spray stability test fails, see Optimizing the Ion Source Parameters. Refer to the instrument manual for instructions.
Calibration > Change Mass Calibration Due Time	By default, the recommended calibration time is 25 hours after the last successful mass calibration. Here, the due time setting ("Recommended Date") for the next mass calibration can be customized. You may consider a longer time period between two succeeding mass calibrations. Mass accuracy is ≤3 ppm within 25 hours (specification). Please evaluate any change in the due time setting. A change in the due time will adjust the recommended date and thus the time point when a warning message appears in the resulting raw data files. ❖ **To change the calibration time** 1. In the Diagnostics pane, click **Change Mass Calibration Due Time**. In the table below, the parameter value becomes visible and shows the current setting. 2. Enter a new validity period (for example, 72—for 3 days). 3. Click **Start** to store the new setting. A green check will appear next to the Parameter in the tree.

Category	Description
Define Scan > Disable AGC mode	Per default, the MS is running with the Automatic Gain Control (AGC) switched on, that is the ion flux from the ion source is constantly monitored and a forecast of the ions to come is made. The forecast can be erroneous in case of a non-continuous ion-flux ion source, such as a MALDI source. Therefore, you can choose between AGC on or off: • 1 : Prescan (default, electrometer is enabled, AGC is on) • 0 : Fixed (electrometer is switched off, AGC is off). The MS will always use the maximum injection time set in the Tune application. The settings are applied by clicking the **Start** button.
Define Scan > Set Multi RF Injection Threshold Ratio	This parameters allows to widen the mass range injected through the (interface) by one single injection. The factor describes the mass range width (between first mass and last mass) that is transferred through the interface by a single injection. With a factor of 4 (default), this allows to transfer from *m/z* 100 to *m/z* 400 or from *m/z* 250 to *m/z* 1000, for example. Range: 1.2–1000 You can access a wider mass range with one single injection by entering a larger value. For example, type “6” and press <Enter>. You can now access from *m/z* 250 to *m/z* 1500 (factor of 6 from first mass setting) with one injection, for example. The settings are applied by clicking the **Start** button. **Tip** The system is optimized for a factor of 4—this it s a reasonable value when using MALDI in non-imaging applications. Keep in mind that the change of the factor to larger values will (usually) sacrifice ion transfer through the interface, particularly for the higher *m/z* values in the interrogated mass ranges transferred by this factor.

Category	Description
Define Scan > External Handshake	Three parameters are available for the external handshake. You can set specific values in the Parameter Value column. • Scan Handshake mode - 0: Off (default) - 1: Handshake - 2: Handshake (MS only) Select **Handshake** to insert a hardware handshake mechanism between scans. In this mode, trigger lines are used to establish a mechanism of scan synchronization with an external device. There is a Ready output signal from the MS and a Trigger input signal to the MS. The external device can start an MS scan (acquisition of a single spectrum) self-timed, but it needs to adhere to the Ready output signal coming from the MS, to not overrun the mass spectrometer timing. • Handshake N-th Counter Input range: 1–1000000, default 1 This parameter is available only when Scan Handshake mode is active. A set value of greater than 1 will insert a handshake only every N-th scan. A set value of, for example, 10 will enable for 10 scans to be subsequently acquired for a single trigger input. The trigger input needs to be set for the first scan of a series only. The other scans (in this example, 9 scans) will also run in absence of the trigger input. This is applied in a continuous MS application like DESI or MALDI in a line scan. • Handshake min. Trigger Delay (msec) Input range: 0–500, default 10 This parameter is available only when Scan Handshake mode is active. It provides an option to reduce the jitter between an external trigger input and the actual injection of ions for the MS scan, in case exact timing between the external trigger input and the actual ion injection event is needed. The settings are applied by clicking the **Start** button.

Category	Description
Define Scan > Diagnostic Trigger out	To synchronize external events (for example, laser pulsing) with scan events that are not individually triggered by a trigger input signal, various states of a scan event can be reported to the external device. • 0: Off (default) • 1: Inject Event • 2: IRM Event; syncs with IRM trapping time, the contact is closed when ions are in the ion-routing multipole. • 3: Acquisition start • 4: PreTrigger; a contact closure is registered on the peripheral panel Digital Out 1B. The diagnostic trigger signal can be measured with an oscilloscope using a circuit with a pull up resistor. The cycle duration of the measured signals fits to the cycle time of the chosen scan event (which depends on the mass resolution setting). For a typical MALDI application, select the value “1” to synchronize laser pulse, desorption/ionization, and ion injection. This output signal can be especially helpful in combination with a Handshake N-th Counter selected larger than 1. The settings are applied by clicking the **Start** button.

4

Method Editor Application

This chapter describes how to use the Method Editor application with the Thermo Scientific™ Orbitrap Exploris MX MS. You create an MS instrument method (combined with the optional autosampler and liquid chromatograph instrument methods) by defining the experiment type and setting various parameters. These include settings for the MS, syringe pump, and divert valve; and the mass ranges and fragmentation transitions for the experiments.

Tip The parameter descriptions for the scan types are built into the application. To see a tooltip description, point to the parameter name, and for additional information, click **Learn More**.

Contents

Menus

The Method Editor application window has the following menus:

- File Menu
- Orbitrap Exploris Menu

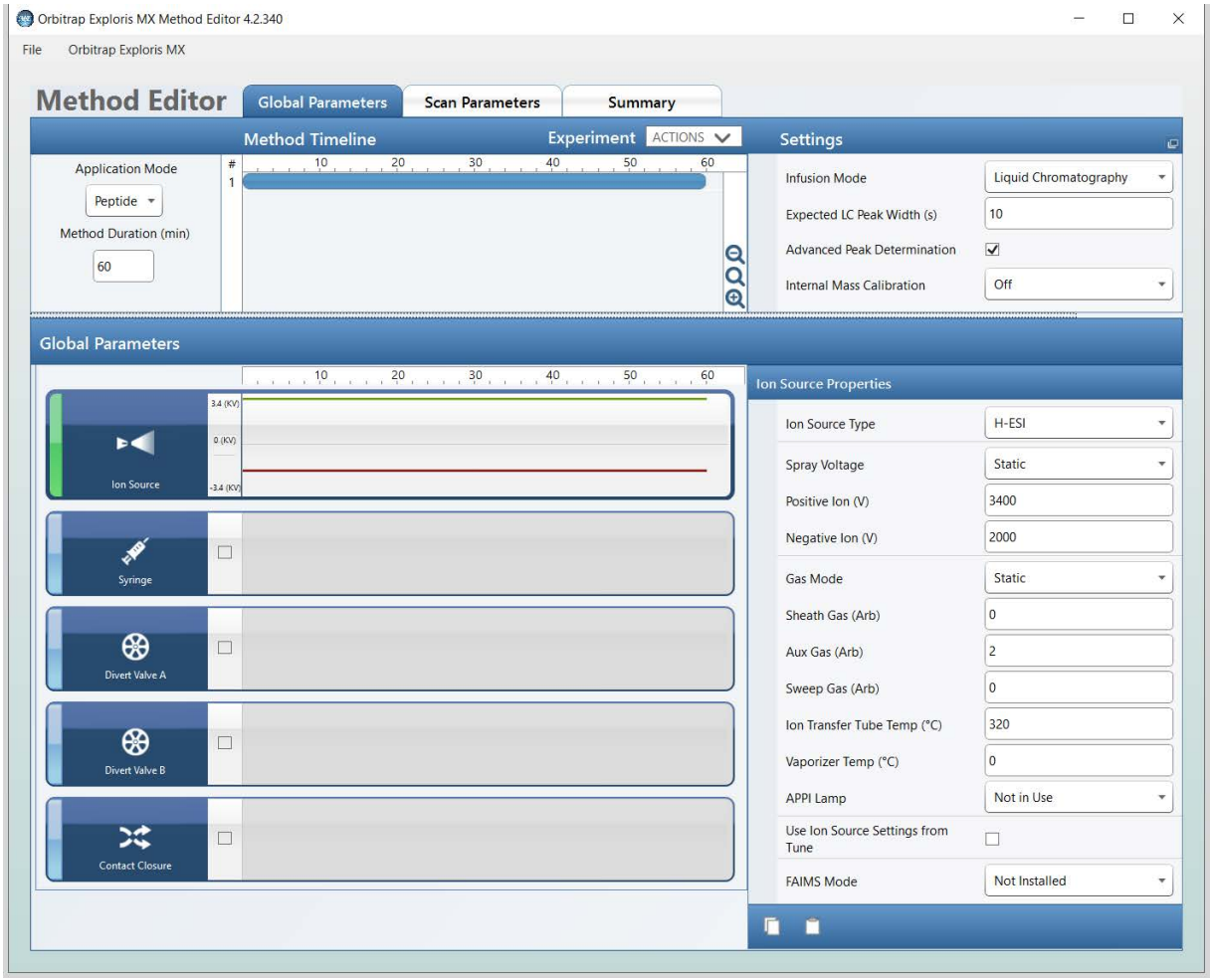


Figure 4-1. Method Editor application window

File Menu

The File menu provides commands for file and program operations. It has the following commands:

Command	Description
New	Creates a new method.
Open	Displays the Open dialog box. Use the Open dialog box to find and open an instrument method file (*.meth) that already exists.
Save	Saves the (changed) settings of the active method. If a new method is created, the Save As dialog box opens.

Command	Description
Save As	Opens the Save As dialog box. Use the Save As dialog box to save the settings of the active method into a new file and to select the location (disk and folder) where you want to save it.
Is Method Modified	Checks if the parameters of the active method are different from the saved file. The result is displayed in a message box.
Validate	Checks if the active method has all parameter settings that are required for it to be executed successfully.
Create Method Summary	Creates a text file that contains all parameter settings of the active method.

Orbitrap Exploris Menu

The Orbitrap Exploris menu provides various import commands. It has the following commands:

Command	Description
Import Method from Raw Data File	Reads the data stored in an Exploris raw data file and creates a method from the information therein.
	IMPORTANT Importing the method from a raw file will replace the contents of the current method. If you do not want to replace the contents of the current method, open a new method before you import the raw file data.
Check for New Templates	In addition to the system templates installed with the Method Editor application, new or updated templates might be available from the Thermo Fisher Cloud, independent from the usual software release cycle. The Method Editor application checks for changes with the system templates when it is launched and when new methods are about to be created. Subscribed product owners or administrators will be notified with the template addition, update or deletion. When you choose this command, a dialog box appears that contains a table with the new templates, if available. To download a new or updated template, select it in the table and click **Update**. You can select several templates by holding the <Shift> or <Ctrl> key while you click. If you want to check manually for updated templates, select the check box at the bottom of the table. You must then choose this command to check for changes.
	Note When an online template is removed by Thermo Fisher Scientific, you are notified to remove it also from the system templates.

Global System Parameters

On the Global Parameters page, you can configure the settings for the ion source, syringe pump, divert valves, and any connected devices controlled by the contact closure signal. The Method Editor application uses these settings for all scans.

Note A red border around a parameter box indicates that the set value is out of range. A yellow border around a parameter box indicates that the set value is outside of the recommended range. Point to the parameter box to display the valid range. The Method Editor displays all changed set values of given parameters in bold type until you save them.

Tip Click the Summary tab to view the global parameter settings.

Global MS Settings

On the top left of the Method Editor, you specify the experiment application mode and the method duration. On the top right side, you select the infusion mode and how to perform the internal mass calibration.

Note To use the EASY-IC™ internal calibration setting, you must activate the internal calibration source in the Foundation Instrument Configuration window. See Configuring the Instrument in Thermo Foundation.

Parameters for the Global MS Settings

Parameter	Description
Note These parameters appear on both the Global Parameters and Scan Parameters pages.	
Application Mode	Displays a list of application modes where each mode has predefined experiment templates. The modes are as follows: • Peptide (default) • Small Molecule • Intact Protein (with BioPharma option)
Method Duration (min)	Defines the method duration in minutes. Range: 0.1–5000

Parameter	Description
Settings	
Pressure Mode	(Application Mode: Intact Protein) Available options are: • Low Pressure (default): Optimal detection for intact protein mass and top-down detection of large fragment ions. • Standard Pressure: Optimal detection for small molecules, bottom-up and top-down protein experiments. • High Pressure: Optimal detection for native protein analysis experiments.
Infusion Mode	Available options are: • Liquid Chromatography (default) Select Liquid Chromatography when the sample is introduced by LC (that is, precursors and precursor intensities change with time). • Infusion Select Infusion when injecting the sample by direct infusion (that is, precursors and precursor intensities do not change with time).
Expected LC Peak Width (s)	(Infusion Mode: Liquid Chromatography) This parameter is used for a variety of features including Maximum Injection Time Mode: Dynamic, Dynamic Exclusion: Auto and scheduling AGC prescans. It is recommended to measure/determine the Expected LC Peak Width(s) from previous runs. It is taken at 10% valley (FWTM)—use Peak width as a first approach. The Expected LC Peak Width(s) has a direct influence on AGC. Please use Peak width of the narrowest peak of the chromatogram. The Expected LC Peak Width(s) measure is used to ensure proper calculations for AGC measures, that is the scheduling of periodic AGC pre-scans and receiving scan-to-scan AGC info. Range: 1–1000
Advanced Peak Determination	(Default) Select the check box to apply the Advanced Peak Determination algorithm. The Advanced Peak Determination (APD) algorithm is an advanced algorithm that improves the determination of the charge states and monoisotopic *m/z* values of isotopic envelopes.

Parameter	Description
Internal Mass Calibration	The internal calibrant source provides an internal reference mass that is analyzed within the same analytical scan of your sample measurements. Internal calibration provides the most accurate corrections to the data. • Off: No lock mass correction is performed. • EASY-IC™: The internal EASY-IC source provides fluoranthene radical ions, which are used as reference masses for positive and negative polarity lock mass correction. • User-defined Lock Mass: One or more *m/z* values can be defined as lock mass(es) to perform a lock mass correction during the run. Lock Mass Injection is not selected per default. When you select this option, the lock mass table appears. (Scroll down to view the table.) If no lock mass is found within one scan, the system will apply the last successful locking information to this scan. The time duration since the last locking and the lock mass correction are provided in the scan header of each individual scan.

Parameter	Description
Mode	(Internal Mass Calibration: EASY-IC™ or User-defined Lock Mass) • Run Start (only with Internal Mass Calibration: EASY-IC™) During the “prepare for run” phase, a lock mass correction is performed via tSIM scans. The replicates are analyzed statistically to exclude outliers and determine the best correction value. The correction is applied to all scans throughout the run. This mode enables the highest acquisition speed. • Scan-to-Scan The lock mass correction is determined in every single scan. This mode delivers the highest mass accuracy. However, for the lock mass injection a certain overhead time is needed. The overhead time for injecting the lock mass (EASY-IC or User-defined Lock Mass) is typically 6 to 10 ms/scan. • Timed Applies the lock mass correction within the retention time window (start/stop) setting. The time window and the polarity is defined in the table that appears when this mode is chosen. The Timed mode provides the ability to refresh the lock mass correction multiple times during the data acquisition of a raw file (run), and thus offers a balance between high mass accuracy and high acquisition speed. The last successful locking information is applied to all subsequent scans until the next timed window applies and a lock mass correction is performed. If no lock mass is found, the last locking information will continue to apply.

Parameter	Description
Lock mass table	(Internal Mass Calibration: User-defined Lock Mass or EASY-IC: Timed) The lock mass table provides the possibility to: • Define User-defined Lock masses • Define time windows during which the lock mass correction (EASY-IC or User-defined Lock Mass) shall be determined. Lists can be imported from (or exported to) a CSV, a TXT, or an XML file. • *m/z*: The lock mass *m/z*. Range: 40–3000 (8000 with a BioPharma license) • t start (only with Mode=Timed): The time (in minutes) to start the lock mass correction determination. Range: 0–Duration of active method; default: 0 • t stop (only with Mode=Timed): The time (in minutes) to stop the lock mass correction detrmination. Range: 0.1–Duration of active method; default: 60 • Polarity: The polarity of the lock mass.
Current Lock Mass	(Internal Mass Calibration: User-defined Lock Mass) Use the list to select an available lock mass list. Click Save to save the active lock mass list. Click Save As to save the active lock mass list under another name. Click Delete to delete the active lock mass list.

Parameter	Description
Mass Tolerance (ppm)	(Internal Mass Calibration: User-defined Lock Mass) Defines the mass tolerance window (in ±ppm) for detecting the lock mass defined in the table. Range: 1–20; default: 15
Lock Mass Injection	(Internal Mass Calibration: User-defined Lock Mass) Lock Mass Injection offers the possibility to inject a defined lock mass (if provided in the solvents or similar) to the ions of the analytical scan into the C-trap and ensures the detection of and locking on the chosen reference mass. In general, a lock mass correction can only be performed if the defined *m/z* value is detected in the performed Orbitrap scan. This means, the mass range of the scan of interest must include the *m/z* value of the lock mass of interest. • If the Lock Mass Injection check box is selected, the lock mass injection will be performed for all scans within the method. • If the Lock Mass Injection check box is clear, you need to make sure that the lock mass is covered by at least one experiment/scan in the method. **Example** Full Scan (*m/z* 100–500), lock mass: 279.1591—the lock mass is covered by the mass range of the Full Scan and a correction will be applied to all other scans. The Lock Mass Injection reduces the acquisition speed due to the associated overhead of about 6–10 ms/scan.

Ion Source Properties Pane and Timeline

Use the Ion Source Properties pane and the timeline to set the ion source parameters. For the time-dependent spray voltage table, you can import the settings from (or export them to) a CSV, a TXT, or an XML file.

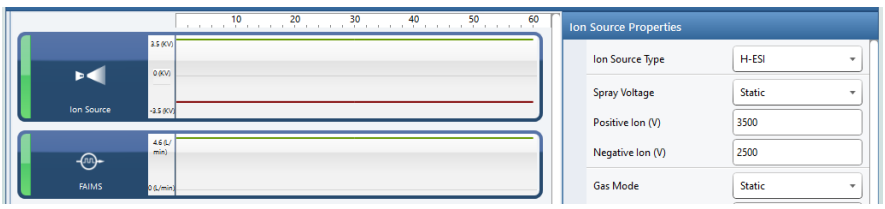


Figure 4-2. Ion Source Properties (FAIMS enabled)

Note If you installed the optional Thermo Scientific FAIMS Pro™ system, the FAIMS parameters appear in this properties pane if you select a FAIMS Mode other than Not Installed.

Tip You can copy () the ion source parameters from the Tune window and paste () them into the Method Editor.

Parameters in the Ion Source Properties Pane

Parameter	Description
Ion Source Type	• NSI (nanoelectrospray ionization) • H-ESI (heated-electrospray ionization) • APCI (atmospheric pressure chemical ionization) • ESI (electrospray ionization) • MALDI (matrix-assisted laser desorption/ionization) • DART (direct analysis in real time)
Spray Voltage Spray Current	• Static: The spray voltage or spray current does not change with time. • Time Dependent: The spray voltage or spray current changes stepwise with time. When you select this option, a table appears where you set the time and either the spray voltage (Ion Source Type: ESI, H-ESI, NSI, MALDI, or DART) or spray current (Ion Source Type: APCI). The Positive Ion and Negative Ion tabs display that polarity mode's settings. - Time (min): The time (in minutes) when the spray voltage/current is changed to the specified value. Range: 0 to method duration - Positive Ion Range: 0–8000 Volts / 0–100 µA - Negative Ion Range: 0–8000 Volts / 0–100 µA
Positive Ion (V)	The spray voltage (in volts) for the positive ion polarity mode. Range (ESI, H-ESI, or MALDI): 0–6000 Range (DART): 0–8000; default: 1000 Range (NSI): 0–3000; default: 1200

Parameter	Description
Negative Ion (V)	The spray voltage (in volts) for the negative ion polarity mode. Range (ESI, H-ESI, or MALDI): 0–5500 Range (DART): 0–8000; default: 1000 Range (NSI): 0–2500; default: 600
Pos Ion Discharge Current (µA)	(Ion Source Type: APCI) The ion discharge current (in microamperes) for the positive ion polarity mode. Range: 0–100; default: 5
Neg Ion Discharge Current (µA)	(Ion Source Type: APCI) The ion discharge current (in microamperes) for the negative ion polarity mode. Range: 0–100; default: 5
Gas Mode	• Static: The gas flows do not change with time. • Time Dependent: The gas flows change with time. When you select this option, a table appears where you can set the time (in minutes) and the flow rates for sheath gas, aux gas, and sweep gas. **Tip** To maximize the table, click the button in the top right corner.
Sheath Gas (Arbitrary)	(Ion Source Type: ESI, H-ESI, APCI, MALDI, NanoCart, or DART) The sheath gas flow rate (in arbitrary units). Range: 0–80
Aux Gas (Arbitrary)	(Ion Source Type: ESI, H-ESI, APCI, MALDI, NanoCart, or DART) The auxiliary gas flow rate (in arbitrary units). Range: 0–25 **Note** If the vaporizer temperature is set to values above 100 °C, the auxiliary gas is automatically set to 5 unless it is set higher manually.
Sweep Gas (Arbitrary)	(FAIMS Mode: Not Installed) The sweep gas flow rate (in arbitrary units). Range: 0–20
Ion Transfer Tube Temp (°C)	The temperature of the ion transfer tube (in degrees Celsius). Range: 0 (ambient temperature) to 400

Parameter	Description
Vaporizer Temp (°C)	(Ion Source Type: H-ESI or APCI) The temperature of the vaporizer tube (in degrees Celsius). Range: 0 (ambient temperature) to 550
APPI Lamp	(Ion Source Type: ESI, H-ESI, or APCI) • Not in Use: The instrument method does not use the APPI lamp. • On: Switches on the installed APPI lamp. • Off: Switches off the installed APPI lamp. Default: Not in Use
	Note • The Method Editor displays the APPI Lamp parameter under the following conditions: - You select a dedicated ion source type in the Instrument Configuration window. - You connect the APPI lamp's USB cable to the instrument. • The MS confirms the state of the APPI lamp before the data acquisition starts. If the ion source does not contain the APPI lamp, the data acquisition application displays an error message.
Use Ion Source Settings from Tune	Uses the source settings that are currently set in the Tune application. Because the instrument method uses the source settings currently applied in the Tune application, the Method Editor application does not display the parameters.

Parameter	Description
FAIMS Mode	If you select a FAIMS Mode other than Not Installed, a FAIMS timeline is displayed in addition to the Ion Source timeline. Choose one of these modes for running methods with FAIMS installed: • Not Installed (default) • Standard Resolution: Provides the best transmission mode by setting the inner and outer electrodes to 100 °C. • High Resolution: Provides twice the resolution of the standard resolution mode by setting the inner electrode to 70 °C and the outer electrode to 100 °C. • User Defined: Displays the fields to enter the electrode temperatures. **Note** The electrode temperatures affect the ion separation. Although the ion transmission might be lower in the FAIMS high resolution mode, the peaks are narrower due to the electrodes' temperature differential.
Total Carrier Gas Flow	This parameter defines the flow of the carrier gas that propels the ions through the electrode space. The optimal gas flow for maximum transmission of ions depends on the type of ion transfer tube and is set as default for this field. In some cases, it might be beneficial to decrease or increase the carrier gas flow to optimize transmission or enhance the spray stability. The timing for dispersing the FAIMS and carrier nitrogen gas: • Static: The gas flow does not change with time. • Time Dependent: The gas flow changes with time as specified in the Total Carrier Gas Flow Table. - Time (min): When the gas flow rate changes to the specified value. Range: 0 to the maximum method duration (5000 maximum) - Gas (L/min): The flow rate for the gas. Range: 0.7–4.3; default: 1.2 This option is often used with higher gas flow rates at the beginning and the end of the chromatographic method to prevent liquid and undesired ions from entering the FAIMS electrode assembly.

Parameter	Description
Total Carrier Gas Flow (L/min)	(Ion Source Type: NSI, H-ESI, APCI, ESI; Total Carrier Gas Flow: Static) The flow rate for the FAIMS and carrier nitrogen gas. The Total Carrier Gas Flow rate should be optimized for each application. At high LC flow rates (500 µL/ min and higher), it can be beneficial to increase the Total Carrier Gas Flow by 0.5–1 L/min. Range: 0.7–4.3; default: 1.2
FAIMS Inner Electrode Temp (°C)	(Ion Source Type: NSI, H-ESI, APCI, ESI; Total Carrier Gas Flow: Static; FAIMS Mode: User Defined) The maximum temperature for the FAIMS inner electrode. Range: 70–100; default: 100
FAIMS Outer Electrode Temp (°C)	(Ion Source Type: NSI, H-ESI, APCI, ESI; Total Carrier Gas Flow: Static; FAIMS Mode: User Defined) The maximum temperature for the FAIMS outer electrode. Range: 70–100; default: 100
Ion Source Properties icons	
Copy 	Copies the ion source parameters to the clipboard.
Paste 	Pastes the ion source parameters from the clipboard.

Syringe Properties Pane and Timeline

Select the Syringe check box to enable the table in the Syringe Properties pane. Then specify the time-dependence of the syringe pump. The Global Parameters page graphically displays the time dependence of the syringe pump on/off status as a timeline. For the syringe position table, you can import the settings from (or export them to) a CSV, a TXT, or an XML file.

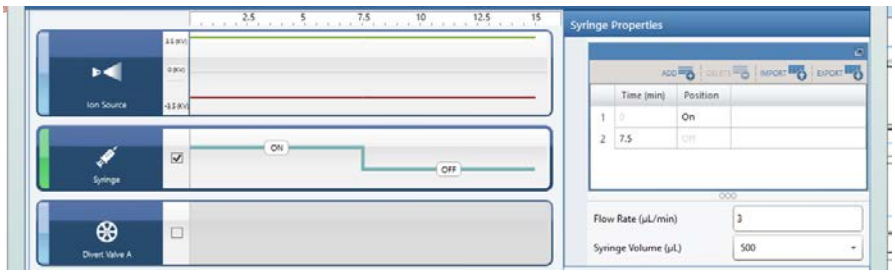


Figure 4-3. Syringe Properties

Parameters in the Syringe Properties Pane

Parameter	Description
Syringe Pump position table	
Time (min)	The time (in minutes) when the syringe pump changes between On and Off, or Off and On. Range: 0 to the maximum method duration (5000 maximum); default: 0
Position	The syringe pump is On or Off at the corresponding time. Default: On
Flow Rate (µL/min)	The volume of solution per unit of time (in micro-liters per minute) that the syringe pump injects (the syringe pump flow rate). Range: 0.5 to 500 (*syringe volume* in µL)/min; default: 3
Syringe Volume (µL)	Values: 50, 100, 250, 500, 1000, 5000, and 10 000; default 500

Divert Valve Properties Pane and Timeline

Select the Divert Valve check box to enable the table in the Divert Valve Properties pane. Then specify the time-dependence of the modular divert/inject valve. The Global Parameters page graphically displays the time dependence of the divert valve position as a timeline. For the divert valve position table, you can import the settings from (or export them to) a CSV, a TXT, or an XML file.

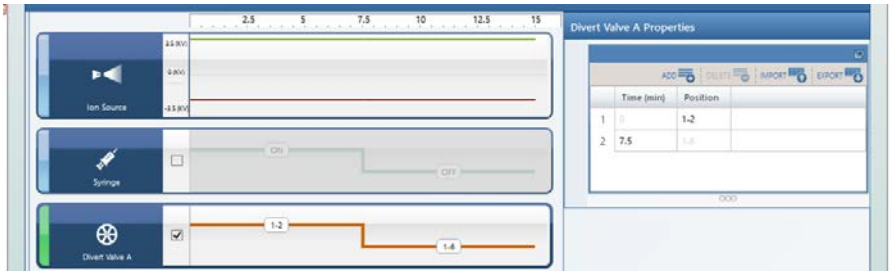
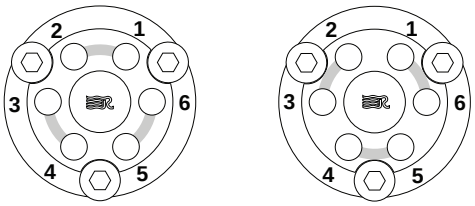


Figure 4-4. Divert Valve Properties

Parameters in the Divert Valve Properties Pane

Parameter	Description
Divert valve position table	
Time (min)	The time (in minutes) when the divert valve changes position. Range: 0 to the maximum method duration (5000 maximum); default: 0
Position	The divert valve position: 1-2 (default) or 1-6.  Position 1–2 Position 1–6 For additional information, refer to the instrument manuals.

Contact Closure Properties Pane and Timeline

Select the Contact Closure check box to enable the table in the Contact Closure Properties pane. Then specify the time dependence of the contact closure on/off signal to an external device. The Global Parameters page graphically displays the time dependence of the contact closure on/off status as a timeline. For the contact closure position table, you can import the settings from (or export them to) a CSV, a TXT, or an XML file.

Note You must configure contact closure in the Foundation Instrument Configuration window. See Configuring the Instrument in Thermo Foundation.

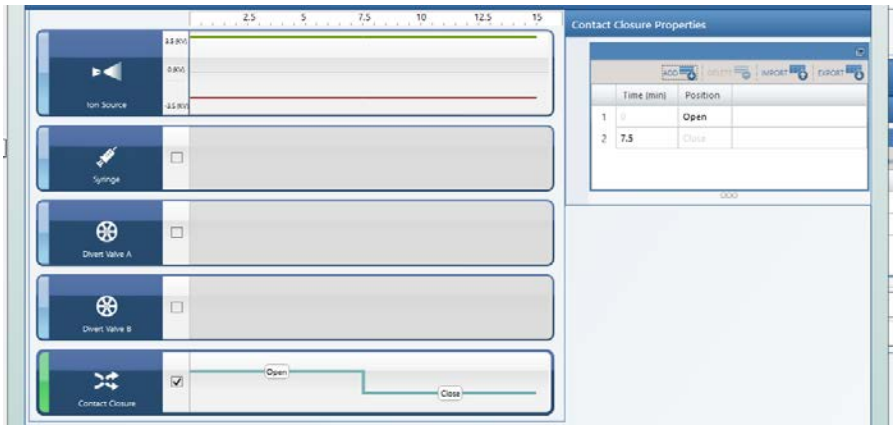


Figure 4-5. Contact Closure Properties

Parameters in the Contact Closure Properties Pane

Parameter	Description
Contact closure position table	
Time (min)	The time (in minutes) when the contact closure state changes. Range: 0 to the maximum method duration (5000 maximum); default: 0
Position	The contact closure signal is Closed or Open. Default: Open

Method Editor Overview

The Method Editor is below the method timeline on the Scan Parameters page. This is where you build the MS instrument method, which can have several experiments, each with its own timeline.

Method Editor Elements

The Method Editor displays the Qualitative View (Qual View toolbar,) in a workflow tree diagram. You can also build a workflow by selecting application-specific System Templates from the Templates View toolbar ( ). These templates describe market-specific typical experiments.

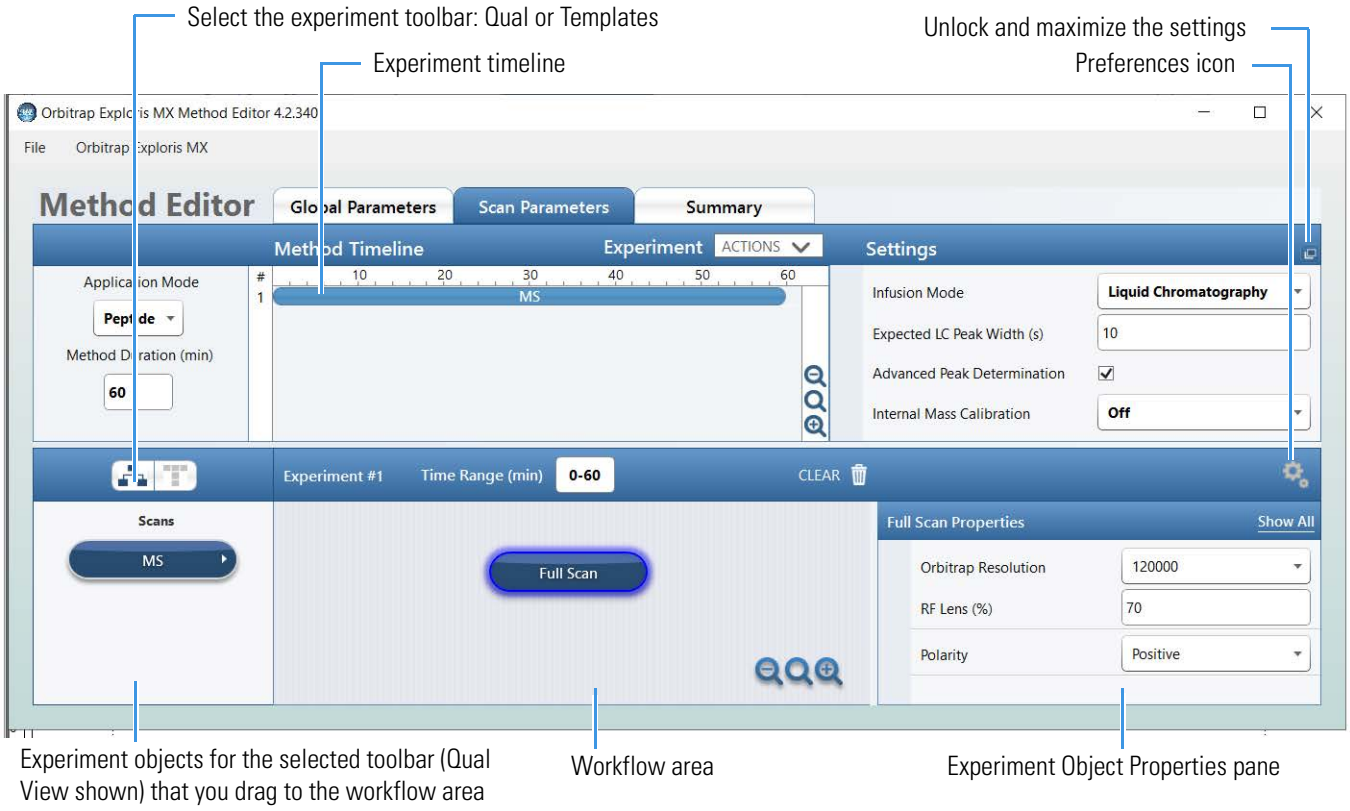


Figure 4-6. Scan Parameters page

Method Timeline

You use the Method Timeline area (at the top of the window) to set the method duration, view experiment timelines, and change the experiment order when there is more than one experiment.

You can enter several experiments to the Method Timeline area.

On the Global Parameters and Scan Parameters pages, the Method Duration box displays the remaining experiment time (in minutes). Where experiments overlap, the MS cycles between them.

The Method Timeline area contains the following parameters and buttons.

Parameter	Description
Method Duration (min)	The time duration (in minutes) for the instrument method. Range: 0.1–5000; default: 60
Experiment Actions	• Add New Experiment • Delete Current Experiment
Buttons	
	• Scroll arrows: When you zoom in on an experiment, these arrows appear if the timeline exceeds the viewing area. • Zoom controls: Zoom Out, Reset Zoom, and Zoom In.

Experiment Workflow Area

Below the Method Timeline area, in the left-side pane of the Scan Parameters page, experiment objects (scan types) are grouped into two experiment toolbars—Qual View (qualitative scans) and Templates View.

You build an experiment workflow by double-clicking or dragging an experiment object into the Method Editor, or by selecting a predefined experiment template that you can modify as needed.

Experiment Controls

This table describes the parameters and buttons that are located above the workflow area.

Parameter or button	Description
Experiment toolbars	Icon for the Qual View ( ): Displays the available experiment objects. Templates View icon ( ): Displays the predefined System Templates for the specified Application Mode. The active view is indicated by a blue (instead of gray) icon.
	(Multiple experiments only) Clicking the left or right arrow displays a specific experiment in the workflow area.

Parameter or button	Description
Time Range (min)	The start and end times (in minutes) for the displayed experiment. The values must be within the specified method duration.
	Clears the contents of the selected experiment without removing the experiment timeline.
	Opens a new window that maximizes the Settings pane.
	The Preferences icon () controls the ON/OFF status of the following: • Enable Recommendations: Shows (or hides) tooltips that specify recommended values or ranges. • Enable Favorites: Shows (or hides) the stars that designate favorite parameters. • Restore Default Favorites: Resets all favorites to the factory setting.

Qual View Workflow Objects

Tip The selected workflow object has a purple border and shadow. Objects that are not selected have a white border. If a border color changes to yellow, one or more of the object's parameter values are not in the recommended range. See Applying Parameter Recommendations. If a border color changes to red, one or more of the object's parameters are out of the operational range. Point to the critical parameter box(es)—highlighted analogously—to see the correct range(s).

This table summarizes how to work with the Qual View workflow objects (scans and filters).

Task	Method
Add an object.	In the experiment toolbar, double-click an icon or drag it into the workflow area (center pane).
Copy an object.	• Right-click the object and choose **Copy**. • (Scans) Drag the scan onto an open node. The object moves only if the new location is appropriate, and the set properties move with the object.
Paste an object.	• Right-click the object under which to paste the copied object, and then choose **Paste**. • Copy an object from one experiment and paste it into another. **Note** For scan objects, the paste function replaces the selected scan.

Task	Method
Delete an object.	• Select the object and press **DELETE**. • Right-click the object and choose **Delete**. • Point to the object, and then click **X** when it appears.
Restore the default settings.	Right-click the object and choose **Restore Defaults** to reset the parameter to the default value.

Setting Method Editor Preferences

This section provides information about handling parameters.

Applying Parameter Recommendations

When you enter a value or range that is not recommended or outside the recommended range for the selected parameter, the Method Editor application changes the border color of the affected workflow objects and parameters to yellow. Point to a yellow parameter box to display the recommended value or range.

❖ **To apply a parameter recommendation or restore the default value**

Do one of the following:

- Right-click the parameter box and choose **Apply Recommended Value**.

  You can choose to ignore the recommendation by choosing **Ignore Recommendation**. When you use the recommended value, the box's border color returns to normal.

- Right-click the workflow object and choose **Restore Defaults,** or right-click a specific parameter box and choose **Restore Default**.

Adding or Removing Parameters From the Favorites List

By default, the Method Editor shows only the preset favorite parameters in the scan properties panes. To add or remove parameters from the favorites list, follow this procedure.

❖ **To modify the favorites list and its display**

1. In the properties pane title bar, click **Show All** if applicable.

   All parameters for the scan type appear.

2. To add or remove a favorite, select the star adjacent to the appropriate parameter (blue is selected and gray is unselected).

3. To show the modified list of favorites, click **Show Favorites**.

Experiment Workflows and Instrument Methods

To create an experiment workflow and instrument method, start by creating an instrument method (METH file) with several experiments—one scan table or workflow diagram and one timeline per experiment.

Tip You can also start with one of the System Templates, which is a complete workflow that you can modify. To view the system templates on the Scan Parameters page, click the **Templates View** icon ( ) and select an Application Mode.

Creating Experiment Workflows (Instrument Methods)

Start on the Global Parameters page.

❖ **To create an experiment workflow**

1. Set the parameters for the ion source, syringe, divert valve, and contact closure.
2. Set the Global System Parameters.

   These parameters are located at the top left and top right of the window.
3. On the Scan Parameters page, do the following:
   a. In the Time Range (min) box, type the experiment's start and end times.

      Tip The Method Duration box displays the latest time of any of the experiments in the saved method. When experiment timelines overlap, the mass spectrometer cycles between them.

   b. On the left side, click the **Qual View** ( ) icon, and then double-click or drag a scan icon to the Place Scan Here node.

      In Qual View, a graphical node (object) appears in the center pane with a purple border to indicate that it is the active node.

   c. To enter a name for the experiment, double-click the experiment timeline. Type the name of the experiment. Press <Enter>.

   d. In the right-side properties pane, set the parameters as required.

      For parameter descriptions, see Qualitative View.

Adding and deleting Experiments in a Method

The instrument method can have several experiments.

❖ **To add an experiment to the method**

In the Experiment Actions list, select **Add New Experiment**.

❖ **To delete an experiment from the method**

1. Go to the experiment by using the arrows above the workflow area.
2. In the Experiment Actions list, select **Delete Current Experiment**.

Saving Instrument Methods

After creating an experiment workflow (instrument method), save it.

❖ **To save the instrument method**

1. Choose **File > Save As**.
2. In the Save As dialog box, enter an instrument method name (.meth extension), and then click **Save**.

Adding Custom Method Templates

If you want to save an instrument method as a template, save it in the Templates pane.

❖ **To add a method template to the custom templates list**

1. After you build your template, select the **Templates View** icon ().
2. Click **Save As Template.**
3. Type a template name and click **Save**.

You can import the template at a later time by selecting My Experiments and selecting the template.

Qualitative View

On the Scan Parameters page, the Method Editor includes qualitative scan types in the left-side Qual View toolbar ( ).

❖ **To add a Qual View scan type to the workflow**

1. Below the Method Duration box, select the **Qual View** icon ( ).
2. Double-click a scan type icon or drag it to the Place Scan Here node.

   When you select a workflow node, its parameters appear in the right-side properties pane.

Tip

- Point to a parameter name to display its description.
- Click the **Summary** tab to view the instrument method settings.

MS (Full) Scan Properties Pane

The MS (Full) Scan Properties pane sets up a full-scan type experiment—that is, signal intensity versus *m/z* over the specified *m/z* range.

Note Changed set values of given parameters appear in bold type. A red table cell or red border around a parameter box indicates that the set value is out of range. Point to the parameter box to display the valid range. If you enter a value that is outside the recommended range, the box border color changes to yellow; see Applying Parameter Recommendations.

Parameters in the Full Scan Properties Pane

Parameter	Description
Orbitrap Resolution	The mass resolution of the Orbitrap analyzer, which is proportional to the inverse square root of the mass-to-charge ratio. Mass resolution is defined as the observed *m/z* value divided by the smallest difference Δ *m/z* for two ions that can be separated: *m/z* / Δ *m/z*. Spectra acquired at higher Orbitrap Resolution allow greater resolution in *m/z* but take longer to acquire. The selected resolution is specified for a peak at *m/z* 200. The available options are: 15 000, 30 000, 60 000, 120 000 (default), and 180 000.

Parameter	Description
Scan Range (*m/z*)	The range (in *m/z*) over which the mass analyzer detects peaks. Range: 40–3000 (40–8000 with BioPharma option); default: 200–3000
	Tip Because the system optimizes the transfer of ions for the defined mass range, we recommend that you restrict the scan range to the region of interest.
FAIMS Voltages	(FAIMS Mode: enabled) Switches On (default) or Off the FAIMS voltages.
FAIMS CV (V)	(FAIMS Voltages: On) The optimized FAIMS compensation voltage. Range: –300 to 300; default 0 For the purpose of harmonization between platforms, the observed CV values on Orbitrap Exploris Series instruments were aligned with those of the Tribrid and TSQ platforms. This means the transmission for one *m/z* should be the same for the same CV setting on all three platforms.
RF Lens (%)	Specify the value to control the RF amplitude applied to the S-lens. Range: 0–200; default: 70 This value is a scaling factor applied to the relationship between the first mass and the RF amplitude. Decreasing the RF level decreases the transmission of high *m/z* ions through the S-lens, increases the transmission of the low *m/z* ions, and might decrease the amount of fragmentation of fragile ions in the S-lens. Increasing the RF level has the opposite effects.
	Tip For stable ions, the default value provides a good starting point. A sample-specific fine tuning of the MS is recommended, however.
AGC Target	Indicates Standard (default) or Custom for the Automatic Gain Control™ (AGC) target value, which controls the number of ions that are injected into the mass analyzer. • Standard: The system sets the recommended target in an automated fashion per scan type and user-defined settings (default). • Custom: You set the AGC Target based on the Standard AGC Target.

Parameter	Description
Normalized AGC Target (%)	(AGC Target: Custom) Specifies the Automatic Gain Control (AGC) target. This is a percentage representing the maximum number of charges to accumulate for a given analysis. Range: 0.01–1000; default: 100 This is the normalized AGC Target value, it is represented as a percentage to aid in calculating the desired AGC Target. The values are as follows: Normalized Base (100%), IRM = 1e6 The IRM fills with ions until it reaches the AGC Target or the maximum injection time. The MS then transfers the ions to the Orbitrap analyzer.
Maximum Injection Time Mode	(Infusion Mode: Liquid Chromatography) Specifies the maximum injection time (max IT) that is allowed to reach the AGC target. The IRM fills with ions until it reaches the AGC target or the max IT. The mass spectrometer then transfers the ions to the Orbitrap analyzer for detection. • Auto: The system calculates the maximum injection time that is available according to the chosen resolution to maximize sensitivity while maintaining the maximum scan rate (parallel acquisition). • Custom: You can specify the maximum injection time. • Dynamic: The system calculates the maximum injection time by dividing the Chromatographic peak width (in msec) by the Desired Minimum Points Across the Peak value. - Minimum value: If the calculated auto max IT for a single target is shorter than the detection duration of the current scan type, the instrument will acquire data in parallel acquisition mode. - Maximum value: If the calculated auto max IT for a single target is longer than the detection duration of the current scan type, the system can apply injection times up to this value, sacrificing optimally parallel acquisition.
Maximum Injection Time (ms)	(Maximum Inject Time Mode: Custom) Maximum time in milliseconds that is allowed to accumulate ions in the IRM until the AGC target is reached. Range: 1–1000; default: 100

Parameter	Description
Desired Minimum Points Across the Peak	(Maximum Injection Time Mode: Dynamic) The minimum number of data points that are required across the peak. This parameter also takes the Expected Peak width into account. When Maximum Injection Time is set to Dynamic, the instrument can dynamically increase the time beyond parallel acquisition while maintaining the number of points across the peak. Range: 1–1000; default: 9
Microscans	Number of scans to average in a given spectrum. Range: 1–10; default: 1 A microscan is one ion injection followed by ion detection. The MS sums microscans to produce one scan, which improves the signal-to-noise ratio of the mass spectral data. **Note** The overall scan time increases linearly with the number of microscans, significantly slowing the rate of spectral acquisition.
Data Type	Indicates how to collect data during the currently selected scan event: • Profile (default): Represents mass spectral peaks as point-to-point plots, with each point having an associated intensity value. • Centroid: Represents mass spectral peaks (as a bar graph) in terms of two parameters: the centroid (the weighted center of mass) and the intensity. The normalized area of the peak provides the mass intensity data. **Tip** Centroiding improves mass spectral data quality, obtains better mass assignments, and reduces the data file size.
Polarity	The polarity mode—Positive (default) or Negative—during a scan to detect ions of that polarity. **Note** The polarity mode applies to an entire experiment, and each experiment in the method can have a different polarity setting.
Source Fragmentation	Select the check box to switch on in-source CID. An offset voltage in the ion source accelerates the ions into the background gas. Collisions with the background gas might aid in the desolvation of the ions and might increase sensitivity.
Energy (eV)	(Source Fragmentation: On) The collision energy (in electron volts) for in-source fragmentation. Range: 1–135; default: 35 If you set the source fragmentation too high, fragmentation of ions might occur.

Parameter	Description
Use EASY-IC™	(Internal Mass Correction: EASY-IC™) If On is selected, it provides an internal reference mass that is used for mass correction during a run.

Using the Experiment Templates

Use the left-side Templates View toolbar ( ) to select predefined, application-specific System Templates. You can then modify the experiment parameters in the properties pane. You can also create a custom workflow template and save it as an EXP file.

For more information about these templates and experiments, and for additional templates, search the Orbitrap Science Library database at www.planetorbitrap.com/library.

Downloading New or Updated System Templates

Download new or updated (revised) system templates for your Orbitrap instrument from the Thermo Fisher Cloud.

By default, each time you open the Method Editor, the system automatically checks for new or updated system templates and notifies if there any are available. You can choose to download any new or updated template that is available. You can save them under new names.

Saving Custom Templates

You can modify system templates and save them under new names.

❖ **To save a custom template**

1. In the Templates View toolbar, click **Save as Template** and browse to the destination folder.
2. Type a name for the template and click **Save**.
3. In the Save Template dialog box, type a template name (.exp extension), and click **Save**.
4. A popup message “Save Method Template” appears.

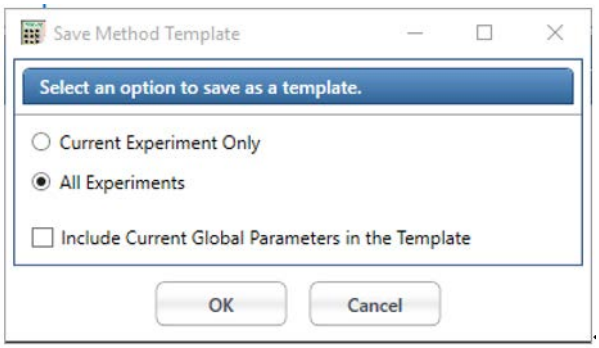


Figure 4-7. Save Method Template dialog box

5. Select an option to save a template:
    - Current Experiment Only: If there are two or more experiments in the method timeline, only the marked experiment is saved as a Method Template.
    - All Experiments: If there are two or more experiments in the method timeline, all experiments in the method timeline are saved as a Method Template.
6. (Optional) Select the check box "Include Current Global Parameters in the Template." The default state is not selected (Only the Scan Parameters of the method are saved). When selected (active), Scan Parameters and Global Parameters (such as ion source settings) are saved in the template.

You can import the template at a later time by selecting My Experiments, and then selecting the template.

System Templates

The System Template folders typically contain multiple system templates, which are divided in template categories.

❖ **To use a system template**

1. Click the left-side Templates View toolbar () to display the available template categories.
2. Click the triangle at the right part of the template category button to display the available system templates.
3. Double-click a system template button or drag it to the Place Scan Here node.
4. If the Global Settings Replacement Options dialog box appears, select an option:
    - Use source settings from the template
    - Keep current source settings

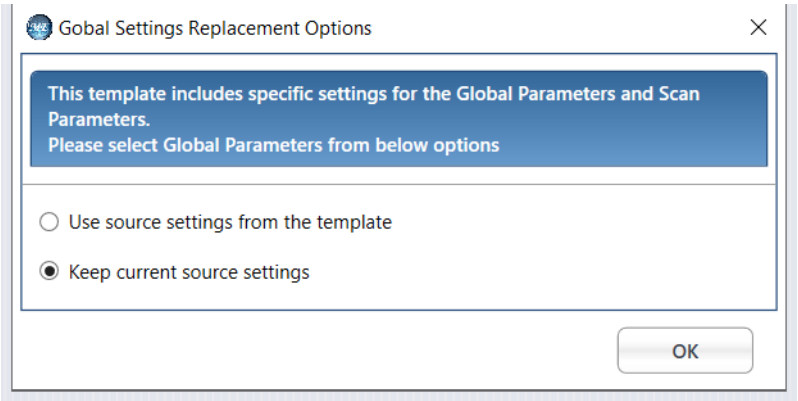


Figure 4-8. Global Settings Replacement Options dialog box

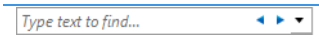
5. Click **OK** to close the dialog box.
6. The workflow area displays the selected experiment.

Available System Templates

When you select an application mode on the Global Parameters or Scan Parameters page, the Method Editor changes the list of displayed system templates.

Summary Page

The Summary page displays the parameters for mass spectrometer setup, syringe pump, divert valves, and contact closure that you specified on the Global Parameters page and the Scan Parameters page.

Button	Description
	Print a summary report.
	Find a word in the Document View.
	Enter the text in the field. Click the down arrow to select a find option. Click the left/right arrows to find the text in the Document View.
	Select the display mode of the Document View: • Single Page Mode • Two Page Mode • Scroll Mode
	Use the slider or click the minus/plus signs to zoom in or out the Document View. Or, position the mouse pointer within the pane, press and hold the <Ctrl> key, and roll the mouse wheel forward to zoom in or backward to zoom out.

❖ To display the Summary page

1. In the Method Editor application window, click the Summary tab.
2. Click the tabs to display the data in a Document View or a Tree View.

Glossary

This section lists and defines terms used in this manual. It also includes acronyms, metric prefixes, symbols, and abbreviations.

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

A

A ampere

AC alternating current

ADC analog-to-digital converter; a device that converts data from analog to digital form.

adduct ion An ion formed by the non-covalent binding of two species, usually an analyte ion and a solvent molecule, and often in the ion source, which contains all the constituent atoms of both species.

AGC target value A value that corresponds to the optimum number of ions in the mass analyzer to avoid space-charge effects. The optimum number of ions produces the best combination of sensitivity, resolution, and mass accuracy.

See also Automatic Gain Control™ (AGC).

All Ion Fragmentation (AIF) Acquisition mode that applies an HCD fragmentation to all ionized molecules without mass filtering.

See also Higher energy Collision-induced Dissociation (HCD).

APCI See atmospheric pressure chemical ionization (APCI).

APCI corona discharge current The ion current carried by the charged particles in the APCI source. The voltage on the APCI corona discharge needle supplies the potential required to ionize the particles. The APCI corona discharge current is set; the APCI corona discharge voltage varies, as required, to maintain the set discharge current.

See also APCI corona discharge voltage.

APCI corona discharge voltage The high voltage that is applied to the corona discharge needle in the APCI source to produce the APCI corona discharge. The corona discharge voltage varies, as required, to maintain the set APCI spray current.

See also APCI spray current.

APCI spray current The ion current carried by the charged particles in the APCI source. The APCI corona discharge voltage varies, as required, to maintain the set spray current.

API See atmospheric pressure ionization (API).

See also:
API ion transfer tube offset voltage
API ion transfer tube temperature.

API ion transfer tube offset voltage A DC voltage applied to the ion transfer tube. The voltage is positive for positive ions and negative for negative ions.

See also API source.

API ion transfer tube temperature The temperature of the ion transfer tube, which should be adjusted for different flow rates.

See also API source.

API source The sample interface between the LC and the mass spectrometer. It consists of the API probe (ESI or APCI) and API stack.

See also:
atmospheric pressure ionization (API)
ESI probe
ESI source.

API tube lens A lens in the API source that separates ions from neutral particles as they leave the ion transfer tube. A potential applied to the tube lens focuses the ions toward the opening of the skimmer and helps to dissociate adduct ions.

See also:
adduct ion
API source
API tube lens offset voltage.

API tube lens offset voltage A DC voltage applied to the tube lens. The value is normally tuned for a specific compound.

See also:
API tube lens
adduct ion
source CID.

AP-MALDI See atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI).

APPI See Atmospheric Pressure Photoionization (APPI).

ASCII American Standard Code for Information Interchange

atmospheric pressure chemical ionization (APCI) A soft ionization technique done in an ion source operating at atmospheric pressure. Electrons from a corona discharge initiate the process by ionizing the mobile phase vapor molecules. A reagent gas forms, which efficiently produces positive and negative ions of the analyte through a complex series of chemical reactions.

See also electrospray ionization (ESI).

atmospheric pressure ionization (API) Ionization performed at atmospheric pressure by using atmospheric pressure chemical ionization (APCI), electrospray ionization (ESI), or nanoelectrospray ionization (nanoESI or NSI).

atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI) Matrix-assisted laser desorption/ionization in which the sample target is at atmospheric pressure.

See also matrix-assisted laser desorption/ionization (MALDI).

Atmospheric Pressure Photoionization (APPI) A soft ionization technique in which an ion is generated from a molecule when it interacts with a photon from a light source.

atomic mass unit Atomic Mass Unit (u) defined by taking the mass of one atom of carbon-12 as being 12u; unit of mass for expressing masses of atoms or molecules.

Automatic Gain Control™ (AGC) Sets the ion injection time to maintain the optimum quantity of ions for each scan. With AGC on, the scan function consists of a prescan and an analytical scan.

See also ion injection time.

autosampler The device used to inject samples automatically into the inlet of a chromatograph.

auxiliary gas The outer-coaxial gas (nitrogen) that assists the sheath (inner-coaxial) gas in dispersing and/or evaporating sample solution as the sample solution exits the APCI, ESI, or H-ESI nozzle.

auxiliary gas flow rate The relative rate of flow of auxiliary gas (nitrogen) into the API source reported in arbitrary units.

B

b bit

B byte (8 b)

base peak The most intense mass peak in the mass spectrum. It is used as the base against which the intensities of all other peaks are normalized.

C

°C degrees Celsius

calibration The process of adjusting a measurement system to deliver results consistent with a known reference.

carrier gas composition (FAIMS) The composition of the carrier gas that transports ions through the FAIMS electrodes. The interaction of the carrier gas affects selectivity and sensitivity. For most analyses, a carrier gas composition of 50:50 He:N_2 is optimal. You must optimize the compensation voltage whenever you change the carrier gas composition.

See also FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy).

carrier gas flow rate (FAIMS) The total gas flow in L/min of the carrier gas. The gas flow rate is from 0 to 5 L/min per gas. The optimal carrier gas flow rate is between 2.5 and 4 L/min, total, with a suggested starting value of 3.5 L/min.

A carrier gas flow rate set too high may cause turbulence in front of the entrance plate. The ion intensities decrease from the optimal value, but the CV of transmission remains unchanged. You must optimize the compensation voltage whenever you change the carrier gas flow rate.

See also FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy).

centroid data Data used to represent mass spectral peaks in terms of two parameters: the centroid (the weighted center of mass) and the intensity. The data is displayed as a bar graph. The normalized area of the peak provides the mass intensity data.

See also centroiding.

centroiding A method used to improve mass spectral data quality, get better mass assignments, and reduce data file size. Profile data is converted into centroid data by a data compression algorithm.

See also:
centroid data
profile data.

charge state The imbalance between the number of protons (in the nuclei of the atoms) and the number of electrons that a molecular species (or adduct ion) possesses. If the species possesses more protons than electrons, its charge state is positive. If it possesses more electrons than protons, its charge state is negative.

chemical ionization (CI) The formation of new ionized species when gaseous molecules interact with ions. The process can involve transfer of an electron, proton, or other charged species between the reactants.

chemical ionization (CI) plasma The collection of ions, electrons, and neutral species formed in the ion source during chemical ionization.

See also chemical ionization (CI).

chromatogram The graphical representation of a chemical separation, such as liquid chromatography, obtained from an analytical instrument called a chromatograph. The result of plotting detector response versus time.

CI See chemical ionization (CI).

CID See collision-induced dissociation (CID).

collision energy The energy used when ions collide with the collision gas.

See also:
collision gas
collision-induced dissociation (CID)
normalized collision energy™

collision gas A neutral gas used to undergo collisions with ions.

collision-induced dissociation (CID) A method of fragmentation where molecular ions are accelerated to high-kinetic energy and then allowed to collide with neutral gas molecules such as helium or nitrogen. The collisions break the bonds and fragment the ions into smaller pieces.

comma-separated values text file A comma-delimited text file. The extension of a comma-separated values text file is .csv. This file format can be read by a text editor program, such as Microsoft Notepad, or by a spreadsheet program, such as Microsoft Excel™.

compensation voltage (FAIMS) A DC potential offset that is applied to the inner electrode of the FAIMS interface to transmit selected subsets of ions through the electrodes. The compensation voltage is tuned for a specific ion. The compensation voltage is typically negative for positive ions and positive for negative ions.

See also FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy).

consecutive reaction monitoring (CRM) scan type A scan type with three or more stages of mass analysis and in which a particular multi-step reaction path is monitored.

CRM See consecutive reaction monitoring (CRM) scan type.

C-Trap curved linear trap

<Ctrl> control key on the terminal keyboard

D

d depth

Da dalton

DAC digital-to-analog converter

DART Direct Analysis in Real Time

Data Dependent experiment A real-time, automated experiment that uses specified criteria to select one or more ions of interest for subsequent analysis, such as MS/MS or ZoomScan.

data-dependent scan A scan mode that uses specified criteria to select one or more ions of interest on which to perform subsequent scans, such as MS/MS or ZoomScan.

DIA Data-Independent Analysis

dispersion voltage (FAIMS) The peak potential of the FAIMS asymmetric waveform. As the dispersion voltage increases, the compensation voltage tends to increase as does the ion intensity. The allowed values are –5000 to –2500 V, and +2500 to +5000 V in increments of 50 V. Standard operating values of the dispersion voltage are –5000 V for positive ions and +5000 V for negative ions. You need to optimize the compensation voltage whenever you change the dispersion voltage.

See also FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy).

divert/inject valve A valve on the mass spectrometer that can be plumbed as a divert valve or as a loop injector.

DS data system

E

EI electron ionization

electrospray ionization (ESI) A soft ionization technique that operates at atmospheric pressure. A solution of the analyte passes through a small capillary so that the fluid sprays through an electric field, generating very fine droplets. The droplets evaporate until all ions are in the gas phase.

See also atmospheric pressure chemical ionization (APCI).

EMBL European Molecular Biology Laboratory

<Enter> Enter key on the terminal keyboard

ESI See electrospray ionization (ESI).

ESI probe A probe that produces charged aerosol droplets that contain sample ions. The ESI probe is typically operated at liquid flows of 1 µL/min to 1 mL/min without splitting. The ESI probe includes the ESI manifold, sample tube, nozzle, and needle.

ESI source Contains the ESI probe and the API stack.

See also:
electrospray ionization (ESI)
ESI probe.

ESI spray current The flow of charged particles in the ESI source. The voltage on the ESI spray needle supplies the potential required to ionize the particles.

ESI spray voltage The high voltage that is applied to the spray needle in the ESI source to produce the ESI spray current. In ESI, the voltage is applied to the spray liquid as it emerges from the nozzle.

See also ESI spray current.

eV Electron Volt. The energy gained by an electron that accelerates through a potential difference of one volt.

expected RT The expected retention time (RT) of a component.

See also retention time (RT).

Extensible Markup Language See XML (Extensible Markup Language).

external lock mass A lock that is analyzed in a separate MS experiment from your sample. If you need to run a large number of samples, or if accurate mass samples will be intermingled with standard samples, you might want to use external lock masses. These allow more rapid data acquisition by eliminating the need to scan lock masses during each scan.

See also internal lock mass.

F

f femto (10^{-15})

°F degrees Fahrenheit

FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy) An optional device for separating ions at atmospheric pressure. FAIMS provides ion separation by taking advantage of compound-dependent changes in ion mobility at high electric field strengths.

See also:
carrier gas composition (FAIMS)
carrier gas flow rate (FAIMS)
compensation voltage (FAIMS)
dispersion voltage (FAIMS)
inner electrode temperature (FAIMS)
outer bias voltage (FAIMS)
outer electrode temperature (FAIMS).

FASTA database A database format that represents either nucleic acid sequences or peptide sequences, and where base pairs or amino acids are represented using single-letter codes. A sequence in FASTA format begins with a single-line description, followed by lines of sequence data. FASTA databases all have the file extension .fasta.

Fast Fourier Transform (FFT) An algorithm that performs a Fourier transformation on data. A Fourier transform is the set of mathematical formulas by which a time function is converted into a frequency-domain function and the converse.

fluoranthene A substance in the ICS that provides both radical cations and anions, which are used in EASY-IC™ as internal reference masses.

forepump The pump that evacuates the foreline. A rotary-vane pump is a type of forepump.

Fourier transform (FT) The mathematical operation that converts the image current signal detected in an ICR trap or Orbitrap mass spectrometer to a set of *m/z* values. The Fourier components correspond to ion mass and the Fourier coefficients correspond to ion abundance.

See also Orbitrap™ mass analyzer.

Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) A technique that determines the mass-to-charge ratio of an ion by measuring its cyclotron frequency in a strong magnetic field.

fragment ion A charged dissociation product of a molecular fragmentation. Such an ion can dissociate further to form other charged molecular or atomic species of successively lower formula weights.

fragmentation The dissociation of a molecule or ion to form fragments, either ionic or neutral. When a molecule or ion interacts with a particle (electron, ion, or neutral species) the molecule or ion absorbs energy and can subsequently fall apart into a series of charged or neutral fragments. The mass spectrum of the fragment ions is unique for the molecule or ion.

FT Fourier Transformation

FT-ICR MS See Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS).

FTMS Fourier Transformation Mass Spectrometry

full-scan type Provides a full mass spectrum of each analyte or parent ion. With the full-scan type, the mass analyzer is scanned from the first mass to the last mass without interruption. Also known as single-stage full-scan type.

FWHM Full Width at Half Maximum

G

Gaussian smoothing A smoothing algorithm that averages each data point with neighboring points to give the displayed value. A Gaussian smoothing uses weighting coefficients corresponding to a Gaussian peak shape.

GC gas chromatograph; gas chromatography

GC/MS gas chromatography / mass spectrometer

GUI graphical user interface

H

h hour

handshake A signal that acknowledges that communication can take place.

HCD See Higher energy Collision-induced Dissociation (HCD).

HCD cell In a linear ion trap, Orbitrap, or hybrid MS, the collision cell where higher energy collision-induced dissociation (HCD) takes place.

See also Higher energy Collision-induced Dissociation (HCD).

header information Data stored in each data file that summarizes the information contained in the file.

heated electrospray See H-ESI.

H-ESI Heated electrospray (H-ESI), a type of atmospheric pressure ionization, converts ions in solution into ions in the gas phase by using electrospray (ESI) in combination with heated auxiliary gas.

See also:
auxiliary gas
electrospray ionization (ESI).

Higher energy Collision-induced Dissociation (HCD) Collision-induced dissociation that occurs in the HCD cell of the Orbitrap™ mass analyzer. The HCD cell consists of a straight multipole mounted inside a collision gas-filled tube. A voltage offset between C-Trap and HCD cell accelerates parent ions into the collision gas inside the HCD cell, which causes the ions to fragment into product ions. The product ions are then returned to the Orbitrap analyzer for mass analysis. HCD produces triple quadrupole-like product ion mass spectra.

High Performance Liquid Chromatography (HPLC) Liquid chromatography in which the liquid is driven through the column at high pressure. Also known as *high pressure liquid chromatography*.

HPLC See High Performance Liquid Chromatography (HPLC).

HRAM High-resolution accurate-mass libraries and compound databases used for analytical software. The HRAM MS/MS spectral fragmentation libraries provide multiple spectra and fragments for every compound with defined retention times for use in targeted screening and quantitation or for unknown analysis in food, environmental, or clinical and toxicological samples.

HV high voltage

Hz hertz (cycles per second)

I

ICD Independent Charge Detector

ICS Internal Calibration Source

image current detection The detection of ion motion by the charge (current) induced on one or more capacitive plates (outer electrodes).

inner electrode temperature (FAIMS) The temperature of the inner FAIMS electrode. Temperature can affect ion separation by changing the gas density within the electrodes. Temperature control enables stable conditions to be reached quickly and maintained indefinitely. The electrodes need to be temperature controlled; otherwise, the compensation voltage changes during system equilibration.

See also FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy).

instrument method A set of experiment parameters that define Xcalibur operating settings for the autosampler, liquid chromatograph (LC), mass spectrometer, divert valve, syringe pump, and so on. Instrument methods are saved as file type .meth.

internal lock mass A lock that is analyzed during the same MS experiment as your sample and is contained in the sample solution or infused into the LC flow during the experiment. Internal lock masses provide the most accurate corrections to the data.

See also external lock mass.

I/O input/output

ion injection time The amount of time that ions are allowed to accumulate in the ion trap mass analyzer when AGC is off. With AGC on, the ion injection time is set automatically (up to the set maximum ion injection time) based on the AGC Target value.

See also Automatic Gain Control™ (AGC).

ion source A device that converts samples to gas-phase ions.

ion sweep gas Extra nitrogen gas that flows along the axis of the API ion transfer tube (between the ion sweep cone and the capillary block) towards the API spray. The sweep gas flow is thus countercurrent to the flow of the ions.

See also ion sweep gas pressure.

ion sweep gas pressure The rate of flow of the sweep gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas out from the Ion Sweep cone towards the API spray.

See also ion sweep gas.

IRM Ion Routing Multipole

K

k kilo (10^3, 1000)

K kilo (2^{10}, 1024)

KEGG Kyoto Encyclopedia of Genes and Genomes

L

LAN local area network

LC See liquid chromatography (LC).

LC/MS See liquid chromatography / mass spectrometry (LC/MS).

LED light-emitting diode

liquid chromatography (LC) A form of elution chromatography in which a sample partitions between a stationary phase of large surface area and a liquid mobile phase that percolates over the stationary phase.

liquid chromatography / mass spectrometry (LC/MS) An analytical technique in which a high-performance liquid chromatograph (LC) and a mass spectrometer (MS) are combined.

lock mass A known reference mass in the sample that is used to correct the mass spectral data in an accurate mass experiment and used to perform a real-time secondary mass calibration that corrects the masses of other peaks in a scan. Lock masses with well-defined, symmetrical peaks work best. You can choose to use internal lock mass or external lock mass.

log file A text file, with a .log file extension, that is used to store lists of information.

M

µ micro (10^{-6})

M mega (10^6)

M^+ molecular ion

matrix-assisted laser desorption/ionization (MALDI) A method of ionizing proteins where a direct laser beam is used to facilitate vaporization and ionization while a matrix protects the biomolecule from being destroyed by the laser.

See also atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI).

MB Megabyte (1 048 576 bytes)

MH^+ protonated molecular ion

microscan One mass analysis (ion injection and storage or scan-out of ions) followed by ion detection. Microscans are summed, to produce one scan, to improve the signal-to-noise ratio of the mass spectral data. The number of microscans per scan is an important factor in determining the overall scan time.

min minute

MRFA A peptide with the amino acid sequence methionine–arginine–phenylalanine–alanine.

MS mass spectrometer; mass spectrometry

MS scan modes Scan modes in which only one stage of mass analysis is performed. The scan types used with the MS scan modes are full-scan type and selected ion monitoring (SIM) scan type.

MS/MS Mass spectrometry/mass spectrometry, or tandem mass spectrometry is an analytical technique that involves two stages of mass analysis. In the first stage, ions formed in the ion source are analyzed by an initial analyzer. In the second stage, the mass-selected ions are fragmented and the resultant ionic fragments are mass analyzed.

MS^n scan mode The scan power equal to 1 to 10, where the scan power is the power *n* in the expression MS^n. MS^n is the most general expression for the scan mode, which can include the following:

- The scan mode corresponding to the one stage of mass analysis in a single-stage full-scan experiment or a selected ion monitoring (SIM) experiment
- The scan mode corresponding to the two stages of mass analysis in a two-stage full-scan experiment or a selected reaction monitoring (SRM) experiment
- The scan mode corresponding to the three to ten stages of mass analysis ($n = 3$ to $n = 10$) in a multi-stage full-scan experiment or a consecutive reaction monitoring (CRM) experiment

See also:
MS scan modes
MS/MS.

multipole A symmetrical, parallel array of (usually) four, six, or eight cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage are applied to the rods to create an electrostatic field that efficiently transmits ions along the axis of the multipole rods.

m/z Mass-to-charge ratio. An abbreviation used to denote the quantity formed by dividing the mass of an ion (in u) by the number of charges carried by the ion. For example, for the ion $C_7H_7^{2+}$, $m/z=45.5$.

N

n nano (10^{-9})

nanoelectrospray ionization (nanoESI or NSI) A type of electrospray (ESI) that accommodates very low flow rates of sample and solvent on the order of 1 to 20 nL/min (for static nanospray) or 100 to 1000 nL/min (for dynamic nanoelectrospray, also called nanoESI nanoLC gradient separation).

See also:
atmospheric pressure chemical ionization (APCI)
electrospray ionization (ESI).

nanoESI (NSI) source The entire nanoelectrospray ion source.

nanoESI (NSI) spray current The flow of charged particles in the nanoESI (NSI) source. The voltage on the NSI spray needle supplies the potential required to ionize the particles.

nanoESI (NSI) spray voltage The high voltage that is applied to the spray needle in the nanoESI (NSI) source to produce the NSI spray current as liquid emerges from the nozzle. The NSI spray voltage is selected and set; the NSI spray current varies.

nanospray ionization (NSI) See nanoelectrospray ionization (nanoESI or NSI).

NCBI (National Center for Biotechnology Information) The organization that provides a Web site for searching through protein and peptide databases. You can also download databases from the NCBI site.

NCE See normalized collision energy™.

neutral loss mass The mass of the neutral species that is lost by the precursor ion in a neutral loss experiment.

See also neutral loss scan mode.

neutral loss scan mode A scan mode that links together an MS and MS/MS scan so that they are scanned at the same rate over scan ranges of the same width. However, the respective mass ranges are offset by a selected mass so that the MS/MS scan is a selected number of mass units lower than the MS scan.

NIST National Institute of Standards and Technology (USA)

normalized collision energy™ For CID in an ion trap, a measure of the amplitude of the resonance excitation RF voltage applied to the endcaps. The normalized collision energy scales the amplitude of the voltage to the precursor mass.

See also collision energy.

NSI (nanoelectrospray ionization) (or nanoESI) A type of electrospray (ESI) that accommodates very low flow rates of sample and solvent on the order of 1 to 20 nL/min (for static nanospray) or 100 to 1000 nL/min (for dynamic nanoelectrospray, also called nanoESI nanoLC gradient separation).

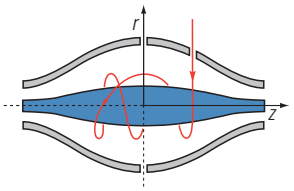
NSI spray voltage The high voltage that is applied to the spray needle in the NSI source to produce the NSI spray current as liquid emerges from the nozzle. The NSI spray current varies.

O

octapole An octagonal array of cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage applied to the rods create an electrostatic field that transmits the ions along the axis of the octapole rods.

offset Used to indicate whether an enzyme cleaves before or after the specified amino acid cleavage sites. An offset of "Before" indicates that the enzyme cleaves before (to the N-terminal side of) the specified amino acid(s). An offset of "After" indicates that the enzyme cleaves after (to the C-terminal side of) the specified amino acid(s).

Orbitrap™ mass analyzer A type of Fourier transform electrostatic ion trap mass analyzer. The Orbitrap mass analyzer consists of a spindle-shaped central electrode surrounded by a pair of bell-shaped outer electrodes. A quadrulogarithmic electrostatic field is generated between these electrodes. Ions inside the mass analyzer orbit in stable trajectories around the central electrode with harmonic oscillations along the length of the electrode. Two detection electrodes record an image current of the ions as they undergo harmonic oscillations. A Fourier transformation extracts different harmonic frequencies from the image current.



An ion's mass-to-charge ratio m/z is related to the frequency f of its harmonic oscillations and to the instrumental constant k by:

$m/z = k/f^2$

OT Orbitrap

See Orbitrap™ mass analyzer.

outer bias voltage (FAIMS) A DC potential that is applied to the outer FAIMS electrode to help transmit ions to the mass spectrometer. Set the outer bias voltage to the same value as the capillary offset.

See also FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy).

outer electrode temperature (FAIMS) The temperature of the outer FAIMS electrode. The electrode temperature can affect ion separation by changing the gas density within the electrodes. The electrodes need to be temperature controlled; otherwise, the compensation voltage changes during system equilibration.

See also FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy).

outlier A calibration data point that does not appear to correlate to other calibration data points within experimental error.

P

p pico (10^{-12})

Pa pascal

peak A maximum in a graph of intensity versus time or intensity versus mass. The position of the maximum is said to be the position of the peak.

peak width The distance across a peak measured at a selected peak-height level, in minutes or mass units. The peak-height level is usually specified as a percentage of the maximum peak height.

See also peak width at half height.

peak width at half height The full width of a peak at half its maximum height, sometimes abbreviated FWHM.

P/N part number

ppm Abbreviation for **p**arts **p**er **m**illion.

precursor ion An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A precursor ion (PR) can be a molecular ion or an electrically charged fragment of a molecular ion. Also known as parent ion.

precursor mass Mass of the corresponding precursor ion or molecule. Also known as parent mass.

product ion An electrically charged product of reaction of a selected precursor ion. In general, product ions have a direct relationship to a particular precursor ion and can correlate to a unique state of the precursor ion.

product mass The mass-to-charge ratio of a product ion. The location of the center of a target product-ion peak in mass-to-charge ratio (*m/z*) units.

See also product ion.

profile data Data representing mass spectral peaks as point-to-point plots, with each point having an associated intensity value.

PrOSA Proportional Orbitrap Signal Adjustment

psig pounds per square inch, gauge

PTM posttranslational modification

Q

quadrupole A symmetrical, parallel array of four hyperbolic rods that acts as a mass analyzer or an ion transmission device. As a mass analyzer, one pair of opposing rods has an oscillating radio frequency (RF) voltage superimposed on a positive direct current (DC) voltage. The other pair has a negative DC voltage and an RF voltage that is 180 degrees out of phase with the first pair of rods. This creates an electrical field (the quadrupole field) that efficiently transmits ions of selected mass-to-charge ratios along the axis of the quadrupole rods.

R

RAM random access memory

raw data Uncorrected liquid chromatograph and mass spectrometer data obtained during an acquisition. Xcalibur and Xcalibur-based software store this data in a file that has a .raw file extension.

***raw* file** A data file that contains the acquired data with the .raw file extension.

See also raw data.

reference peak In spectra from high resolution analyses, a peak (R) from an internal reference compound that has a known, precise mass. Reference peaks are used as measures of calibration accuracy.

resolution The ability to distinguish between two points on the wavelength or mass axis.

retention time (RT) The time after injection at which a compound elutes. The total time that the compound is retained on the chromatograph column.

RF voltage An AC voltage of constant frequency and variable amplitude that is applied to the ring electrode or endcaps of the mass analyzer or to the rods of a multipole. Because the frequency of this AC voltage is in the radio frequency (RF) range, it is referred to as RF voltage.

RMS root mean square

ROM read-only memory

rotary-vane pump A mechanical vacuum pump that establishes the vacuum necessary for the proper operation of the turbomolecular pump. (Also called a roughing pump or forepump.)

RS-232 An accepted industry standard for serial communication connections. This Recommended Standard (RS) defines the specific lines and signal characteristics used by serial communications controllers to standardize the transmission of serial data between devices.

RT An abbreviated form of the phrase retention time (RT). This shortened form is used to save space when the retention time (in minutes) is displayed in a header, for example, RT: 0.00-3.75.

S

s second

scan mode and scan type combinations A function that coordinates the three processes in the MS: ionization, mass analysis, and ion detection. You can combine the various scan modes and scan types to perform a wide variety of experiments.

selected ion monitoring (SIM) scan type A scan type in which the mass spectrometer acquires and records ion current at only one or a few selected mass-to-charge ratios.

See also selected reaction monitoring (SRM) scan type.

selected reaction monitoring (SRM) scan type A scan type with two stages of mass analysis and in which a particular reaction or set of reactions, such as the fragmentation of an ion or the loss of a neutral moiety, is monitored. In SRM a limited number of product ions is monitored.

serial port An input/output location (channel) for serial data transmission.

sheath gas The inner coaxial gas (nitrogen), which is used in the API source to help nebulize the sample solution into a fine mist as the sample solution exits the ESI or APCI nozzle.

sheath gas flow rate The rate of flow of sheath gas into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of sheath gas to the ESI or APCI nozzle.

sheath gas pressure The rate of flow of sheath gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of inner coaxial nitrogen gas to the ESI or APCI nozzle. A software-controlled proportional valve regulates the flow rate.

See also sheath gas.

signal-to-noise ratio (S/N) The ratio of the signal height (S) to the noise height (N). The signal height is the baseline-corrected peak height. The noise height is the peak-to-peak height of the baseline noise.

SIM See selected ion monitoring (SIM) scan type.

source CID A technique for fragmenting ions in an atmospheric pressure ionization (API) source. Collisions occur between the ion and the background gas, which increase the internal energy of the ion and stimulate its dissociation.

SRM See selected reaction monitoring (SRM) scan type.

sweep gas Nitrogen gas that flows out from behind the sweep cone in the API source. Sweep gas aids in solvent declustering and adduct reduction.

See also sweep gas flow rate.

sweep gas flow rate The rate of flow of sweep gas into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas to the sweep cone of the API source.

See also sweep gas.

syringe pump A device that delivers a solution from a syringe at a specified rate.

T

target compound A compound that you want to identify or quantitate or that a specific protocol (for example, an EPA method) requires you look for. Target compounds are also called *analytes,* or *target analytes*.

TIC See total ion current (TIC).

Torr A unit of pressure, equal to 1 mm of mercury and 133.32 Pa.

total ion current (TIC) The sum of the ion current intensities across the scan range in a mass spectrum.

tube lens offset The voltage offset from ground that is applied to the tube lens to focus ions toward the opening of the skimmer.

See also source CID.

Tune Method A defined set of mass spectrometer tune parameters for the ion source and mass analyzer. Tune methods are defined by using the instrument software's tune window and saved as tune file.

A tune method stores tune parameters only. (Calibration parameters are stored separately, not with the tune method.)

tune parameters Instrument parameters whose values vary with the type of experiment.

TWA time weighted average

U

u atomic mass unit

ultra-high performance liquid chromatography (U-HPLC) See High Performance Liquid Chromatography (HPLC).

V

V volt

V AC volts alternating current

V DC volts direct current

W

W watt

WEEE European Union Waste Electrical and Electronic Equipment Directive. Provides guidelines for disposal of electronic waste.

X

XML (Extensible Markup Language) A general-purpose markup language that is used to facilitate the sharing of data across different information systems, particularly via the Internet.

Index

Symbols

A

B

C

D

E

F

G

H

I

L

M

O

P

R

S

T

V

W

ThermoFisher
SCIENTIFIC

thermo scientific